

Supporting information

DFT studies on the mechanism of alcohol oxidation by (bpy)Cu^I-TEMPO/NMI catalytic system

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Table S1 Cartesian coordinates all structures considered in this work (B3LYP level)

0 Charge=1 Multiplicity = 1	0 Charge=1 Multiplicity = 3
Cu -0.00001200 1.42799300 -0.00116500	Cu -0.00173800 1.42825200 -0.00037700
N -1.31256800 -0.00050200 -0.00084500	N -1.31524100 -0.00077300 -0.00081900
N 1.31257000 -0.00048000 -0.00083400	N 1.31564800 0.00303300 0.00011700
C -1.53295400 -2.38197900 0.00093700	C -1.52702600 -2.38357000 0.00065600
C -0.74314900 -1.23388000 0.00008400	C -0.74153000 -1.23227300 -0.00003800
C -3.49366700 -0.98063200 -0.00024600	C -3.49304000 -0.99063100 -0.00017300
H -3.54965800 -3.13793900 0.00143000	H -3.54040900 -3.14825000 0.00113600
H -3.03510900 1.13950500 -0.00176000	H -3.04346000 1.13057800 -0.00143700
H -4.56880800 -0.84053800 -0.00041500	H -4.56871000 -0.85459900 -0.00022700
H -1.08119200 -3.36678000 0.00172700	H -1.07161200 -3.36664600 0.00131500
H 3.54971000 -3.13788300 0.00143600	H 3.54981000 -3.13809400 -0.00003500
C 2.92270200 -2.25182200 0.00077600	C 2.92399400 -2.25118900 0.00001400
C 3.49368500 -0.98057700 -0.00023200	C 3.49627700 -0.98061700 0.00013300
C 1.53299500 -2.38195400 0.00093700	C 1.53425100 -2.37916400 -0.00006700
C 2.64869000 0.12545600 -0.00101200	C 2.65217600 0.12603200 0.00013000
H 4.56882400 -0.84046500 -0.00039600	H 4.57155500 -0.84152100 0.00019500
C 0.74317200 -1.23386800 0.00008600	C 0.74545500 -1.23012500 -0.00000700
H 1.08124800 -3.36676300 0.00171800	H 1.08159400 -3.36350400 -0.00025300
C -2.92266300 -2.25186700 0.00077000	C -2.91713100 -2.25956100 0.00058400
H 3.03509500 1.13955300 -0.00174300	H 3.04067100 1.13928200 0.00018700
C -2.64869000 0.12541400 -0.00102500	C -2.65209700 0.11843100 -0.00082400
O 0.66006400 3.23004400 0.00223300	O 0.65014100 3.23836000 -0.00062200
O -0.66012500 3.23003400 0.00240200	O -0.66262400 3.23459400 0.00218700
1 Charge=1 Multiplicity = 1	1 Charge=1 Multiplicity = 3
Cu -0.80801200 -0.78586600 -0.42017400	Cu -0.78461700 -0.80566800 -0.35718500
N -2.66620800 -0.66070300 0.15258100	N -2.68033700 -0.65360700 0.15684200
N -0.90349900 1.18720500 -0.39407800	N -0.88050100 1.17594000 -0.38146800
C -4.43618500 0.85506000 0.68194900	C -4.44572000 0.89680700 0.60115500
C -3.12099500 0.60965300 0.29220800	C -3.12291400 0.62433000 0.25500700
C -4.80770900 -1.52485200 0.75707000	C -4.85340900 -1.47400900 0.72212600
H -6.31376400 -0.05094000 1.22254400	H -6.35116400 0.03105600 1.10926700
H -3.04415900 -2.68211100 0.20845500	H -3.10115200 -2.66883900 0.24674000
H -5.44167600 -2.38827200 0.92514700	H -5.50335700 -2.32508200 0.89214700
H -4.80213000 1.86860400 0.79599000	H -4.80090700 1.91738800 0.68029600

H	-1.51282500	4.99050400	-0.21976700	H	-1.47286400	4.98563800	-0.28944200
C	-1.33755300	3.92039100	-0.26933600	C	-1.30189900	3.91399000	-0.31586500
C	-0.09788400	3.42279100	-0.66767200	C	-0.05454200	3.40339500	-0.67084400
C	-2.35901900	3.03072600	0.06383500	C	-2.33657300	3.03510400	0.00467700
C	0.07918800	2.04292100	-0.71349400	C	0.11484800	2.02181000	-0.68661500
H	0.71799600	4.08344900	-0.93894700	H	0.77239300	4.05497200	-0.93048700
C	-2.11636100	1.65944400	-0.00867300	C	-2.09963200	1.66112200	-0.03779000
H	-3.32710400	3.40680400	0.37283400	H	-3.30991600	3.42250000	0.28125700
C	-5.28648400	-0.22647400	0.91886800	C	-5.31823200	-0.16586600	0.83978200
H	1.02058400	1.59426500	-1.01313100	H	1.06312300	1.56459400	-0.95058100
C	-3.48235400	-1.70283600	0.36736400	C	-3.52066400	-1.67578500	0.37191500
O	0.07749900	-3.32115700	-0.76946000	O	0.16083700	-3.23866300	-1.17110700
O	-0.92159700	-2.51174400	-1.07147100	O	-0.95161500	-2.59653200	-0.96220100
O	1.17654800	-0.96091800	-0.36362600	O	1.14962000	-1.07608200	-0.15404400
C	1.83520500	-0.97382300	0.94740900	C	1.84517500	-0.97045300	1.12571200
H	1.55805700	-0.02098000	1.40743300	H	1.56669700	0.01138000	1.52018100
C	3.34394300	-1.10905700	0.81230200	C	3.35208300	-1.09180500	0.95299000
H	3.75513100	-1.20125400	1.82591900	H	3.79870900	-1.09869600	1.95572900
H	3.57649800	-2.05665700	0.30610200	H	3.58570100	-2.07052600	0.51090900
C	4.02197600	0.06693200	0.08404100	C	3.98321500	0.03571500	0.11442200
H	3.56663300	0.17393100	-0.91181600	H	3.49168200	0.05796100	-0.86963300
H	3.81667500	0.99742100	0.63181300	H	3.77944200	1.00198600	0.59730200
C	5.50936700	-0.12194600	-0.05422400	C	5.46824300	-0.13795400	-0.06298400
H	5.82944000	-0.97316700	-0.65822200	H	5.78322500	-1.02435400	-0.61699300
C	6.43419600	0.66027400	0.50875000	C	6.39731400	0.69647700	0.41105200
H	6.10502700	1.51004100	1.11109000	H	6.07342000	1.58100800	0.96422700
C	7.91858600	0.47828300	0.38306500	C	7.87968700	0.52974700	0.24591200
H	8.38808500	1.36225800	-0.06806300	H	8.31758200	1.38771800	-0.28091500
H	8.38458700	0.34501300	1.36816900	H	8.38151100	0.47199300	1.22070600
H	8.16905700	-0.39145700	-0.23282200	H	8.12466600	-0.37633700	-0.31757200
H	1.41079600	-1.79338800	1.53834000	H	1.45686700	-1.74149200	1.80173700
H	1.31628500	-1.84383000	-0.77987400	H	1.23150600	-2.00036600	-0.51922600
TS1-2 Charge=1 Multiplicity = 1				TS1-2 Charge=1 Multiplicity = 3			
Cu	-0.72747000	-0.76013900	-0.12739900	Cu	-0.44525100	-0.14804100	0.38464600
N	-2.66570300	-0.68421300	0.02608800	N	-2.00567400	-1.19952300	-0.22530000
N	-0.87249900	1.18305000	-0.14661500	N	-1.69554000	1.36890500	0.17166500
C	-4.52361900	0.79807000	0.29868000	C	-4.29216700	-1.04073900	-0.91216400
C	-3.16036400	0.57906500	0.11646500	C	-3.10137700	-0.44750000	-0.49463700
C	-4.86243300	-1.58645200	0.28328800	C	-3.21828500	-3.18994000	-0.75963200
H	-6.44784500	-0.14265000	0.52677500	H	-5.26788500	-2.90438200	-1.37338700
H	-3.02049000	-2.71402300	0.01422500	H	-1.16054300	-3.07743700	-0.08483500

H	-5.49886900	-2.46235600	0.34043800	H	-3.22487100	-4.27061300	-0.84740700
H	-4.91559000	1.80542900	0.37543200	H	-5.16848300	-0.43905500	-1.12208100
H	-1.53501000	4.97302800	-0.21094800	H	-4.33425200	4.08196700	-0.55274300
C	-1.34554700	3.90429400	-0.19514900	C	-3.58825500	3.32051200	-0.34792400
C	-0.05117000	3.41242100	-0.35179400	C	-2.32984100	3.67328000	0.13629600
C	-2.40612600	3.01187500	-0.02780700	C	-3.88422100	1.97642700	-0.57360100
C	0.14733600	2.03390800	-0.32430100	C	-1.40562500	2.66136500	0.37872400
H	0.79355100	4.07663000	-0.49647000	H	-2.06171000	4.70770100	0.31998000
C	-2.14116900	1.64423700	-0.01175200	C	-2.91360500	1.01177800	-0.30371600
H	-3.41903100	3.38231700	0.07800700	H	-4.85631500	1.69217900	-0.95845100
C	-5.38307400	-0.29838800	0.38426200	C	-4.34802600	-2.42783500	-1.04928400
H	1.12115900	1.57455000	-0.45382400	H	-0.40682500	2.87500800	0.74287600
C	-3.49011500	-1.74062300	0.10298200	C	-2.06365500	-2.53400000	-0.34086400
O	0.16753900	-3.07805500	-1.04685300	O	0.78878700	-2.48196100	1.51922900
O	-0.72021700	-2.63053400	-0.11708800	O	-0.04508100	-1.45666700	1.84739300
H	0.95347600	-2.46948400	-0.85131200	H	1.65877400	-2.05162900	1.35341200
O	1.10488300	-0.84500600	-0.28267600	O	1.20837000	0.47950300	0.13487600
C	1.78457400	-0.84527100	0.96893100	C	2.16129600	0.87076500	1.08889400
H	1.61634100	0.11171000	1.49169500	H	2.30952700	1.96129900	1.02226200
C	3.29000400	-1.04560700	0.75761700	C	3.51583900	0.18515000	0.81964100
H	3.75715000	-1.13237800	1.74714800	H	4.20492600	0.48290300	1.62033600
H	3.45121000	-2.00658200	0.25067200	H	3.39189700	-0.90676000	0.91431200
C	3.96182500	0.08774400	-0.03783600	C	4.12190000	0.51774600	-0.55400600
H	3.45881200	0.17420800	-1.01195500	H	3.39824000	0.23824700	-1.33217300
H	3.81074400	1.04052800	0.49016200	H	4.26402300	1.60388300	-0.62997700
C	5.43413500	-0.14705600	-0.24148700	C	5.43175900	-0.18609500	-0.77989800
H	5.70032400	-1.02716600	-0.83040700	H	5.39212700	-1.27714900	-0.81528200
C	6.40978300	0.62338800	0.24906500	C	6.61421500	0.42206200	-0.92728600
H	6.13688100	1.50157900	0.83859700	H	6.64809600	1.51295900	-0.89264300
C	7.87987100	0.39082400	0.05627100	C	7.92545700	-0.27079700	-1.15202500
H	8.35342900	1.24490000	-0.44575200	H	8.37957300	0.04367000	-2.10099300
H	8.39125700	0.27261200	1.02074900	H	8.64605200	-0.01757900	-0.36305800
H	8.07242000	-0.50495700	-0.54302600	H	7.81124400	-1.35948600	-1.17344900
H	1.40303400	-1.65154600	1.61639200	H	1.82812100	0.63170900	2.11093700
2				2			
Charge=1 Multiplicity = 1				Charge=1 Multiplicity = 3			
Cu	-0.63512200	-0.71778400	-0.20164400	Cu	-0.57498700	-0.69434700	-0.01193400
N	-2.50203700	-0.62629800	0.35294800	N	-2.57163800	-0.78132500	0.10652700
N	-0.84708700	1.21187600	-0.32950500	N	-0.97119700	1.27123900	-0.12773900
C	-4.36221800	0.82557100	0.73861800	C	-4.58741800	0.50589900	0.07228800
C	-3.03526500	0.62253900	0.36938800	C	-3.19539400	0.41963600	0.03036700
C	-4.57804700	-1.55010400	1.07539700	C	-4.68500900	-1.89078700	0.26859400
H	-6.17859400	-0.13588000	1.38383900	H	-6.42233900	-0.60954100	0.22971700

H	-2.73812000	-2.64516400	0.65560900	H	-2.73040000	-2.83104300	0.25378400
H	-5.15237200	-2.42865700	1.34708500	H	-5.23384800	-2.82111700	0.36300600
H	-4.78553300	1.82326900	0.75100200	H	-5.08460400	1.46643900	0.00811700
H	-1.54818900	4.98595800	-0.53329100	H	-2.06075400	4.96502900	-0.26076900
C	-1.34807700	3.92056800	-0.47613100	C	-1.75021300	3.92560400	-0.22114900
C	-0.08475900	3.42018600	-0.78600100	C	-0.39873200	3.58740000	-0.25288000
C	-2.36142200	3.04196200	-0.08857700	C	-2.70748600	2.91540200	-0.12931500
C	0.13012900	2.04648600	-0.69841000	C	-0.05002800	2.24026900	-0.19707500
H	0.72500400	4.07414800	-1.08944800	H	0.37390700	4.34565200	-0.31495100
C	-2.08318300	1.67895000	-0.02205800	C	-2.28662500	1.58609500	-0.08161400
H	-3.34817900	3.41742500	0.15648800	H	-3.76056400	3.16752800	-0.08976700
C	-5.14190700	-0.27643900	1.09431900	C	-5.33865800	-0.66209300	0.19462500
H	1.08125600	1.57058900	-0.91648400	H	0.98224800	1.90868500	-0.19435100
C	-3.24460100	-1.68738500	0.69551500	C	-3.29442100	-1.90541400	0.21587000
O	-1.11761000	-2.82679700	-1.47782300	O	0.73158200	-2.78477200	-1.26373700
O	-0.62194700	-2.51612900	-0.18284700	O	-0.52910300	-2.31853600	-0.91955500
H	-0.31036700	-3.12972900	-1.93971100	H	0.53050200	-3.66939700	-1.63118700
O	1.09848500	-0.58422800	-0.56919200	O	0.99901500	-0.44183300	0.85990100
C	2.01465800	-1.65717000	-0.52115500	C	1.97919700	-1.38082800	1.19281000
H	1.94337800	-2.20358900	0.42857700	H	2.22038400	-1.24171000	2.25854200
C	3.43418400	-1.07873100	-0.67478700	C	3.27366300	-1.18062000	0.36670800
H	4.11806000	-1.93186400	-0.77638200	H	3.96411900	-1.98669300	0.64756500
H	3.48677500	-0.51813200	-1.61691100	H	3.03427300	-1.32076500	-0.69441900
C	3.88008800	-0.19431500	0.50241900	C	3.94270700	0.18511700	0.59460200
H	3.16048200	0.62974300	0.61686500	H	3.22499800	0.97547400	0.32923900
H	3.83860000	-0.77695300	1.43246300	H	4.17055800	0.31182400	1.66084100
C	5.26758200	0.35417800	0.30645000	C	5.19601700	0.32684600	-0.22030600
H	5.40797300	1.00569100	-0.55911000	H	5.07119300	0.30527500	-1.30497700
C	6.31641200	0.08800900	1.09109600	C	6.43233900	0.44935400	0.28493100
H	6.17162100	-0.56689700	1.95287900	H	6.55288900	0.46448100	1.36988100
C	7.70519900	0.62212500	0.89587800	C	7.68898700	0.57915500	-0.52099800
H	8.03245800	1.20259400	1.76863900	H	8.21019200	1.51793500	-0.29042200
H	8.42900800	-0.19478300	0.77570700	H	8.39222200	-0.23081200	-0.28490600
H	7.77107800	1.26735500	0.01363800	H	7.48763600	0.55479000	-1.59675600
H	1.83400000	-2.36978500	-1.34075900	H	1.62634800	-2.41047300	1.03874700
3				3			
Charge=1 Multiplicity = 2				Charge=1 Multiplicity = 4			
C	0.92013600	1.08209600	2.51437600	C	-0.51776200	-2.67641600	1.32589900
C	0.83110200	1.92930100	3.61744800	C	-0.41671100	-3.73457500	2.22693800
C	0.32241300	3.21337900	3.43373400	C	0.83322200	-4.31368700	2.43664800
C	-0.07265500	3.61740100	2.15854400	C	1.93882700	-3.82585100	1.74015800
C	0.04690100	2.71982200	1.09833700	C	1.76392600	-2.76203300	0.85414000
N	0.53434300	1.47395900	1.29810100	N	0.54695000	-2.20130500	0.66819000

H	0.23757300	3.89918400	4.27098300	H	0.94986900	-5.14230000	3.12833600
H	1.30793700	0.06914900	2.56370900	H	-1.45863900	-2.18992300	1.09368300
H	1.15499100	1.58213700	4.59227500	H	-1.30068400	-4.09373400	2.74242500
H	-0.46046100	4.61631400	1.99594900	H	2.91356000	-4.27801900	1.88148700
H	-1.45141900	5.29388700	-2.52612900	H	6.15841000	-2.18998200	-0.69501500
C	-1.05510300	4.35916100	-2.14179600	C	5.11052400	-1.90887100	-0.73343600
C	-0.78909600	3.29450400	-2.99979900	C	4.67274600	-0.92061600	-1.61366100
C	-0.80479600	4.21533900	-0.77738700	C	4.18861400	-2.53826200	0.10125700
C	-0.28766500	2.11126800	-2.46064000	C	3.31929900	-0.59483700	-1.62494500
H	-0.96706300	3.36735600	-4.06688200	H	5.35981600	-0.41091500	-2.28000200
C	-0.29332000	3.00733900	-0.30610900	C	2.84548900	-2.16372300	0.03436800
H	-1.00265000	5.03377900	-0.09500400	H	4.51587200	-3.30598900	0.79251500
N	-0.04510700	1.98020200	-1.15327100	N	2.43413100	-1.20157100	-0.82403800
H	-0.06547300	1.23604500	-3.06273900	H	2.91764200	0.16519300	-2.28576100
Cu	0.58612100	0.30367800	-0.30118800	Cu	0.49562900	-0.74994300	-0.74987400
H	-4.16101700	-3.05765300	2.37666800	H	0.77665400	3.35330400	3.63838900
C	-4.14989000	-2.40145700	1.49924000	C	0.94427200	3.48811800	2.56402500
C	-4.61472000	-3.17802200	0.25087100	C	0.14211300	4.70025900	2.04963800
C	-2.74241300	-1.77937800	1.40162700	C	0.62961000	2.14384800	1.87458200
H	-4.85886400	-1.59641800	1.72195400	H	2.01756700	3.67709600	2.45118100
H	-5.70833500	-3.14078500	0.20806800	H	0.74632400	5.60121700	2.19815500
C	-4.00720200	-2.63741100	-1.06097100	C	-0.27157500	4.56863800	0.56911100
H	-4.35565900	-4.23786400	0.34498300	H	-0.76024700	4.84245900	2.65327700
N	-2.64940600	-0.97537300	0.13627300	N	0.72376700	2.33081900	0.38639600
C	-3.58759700	-1.15379000	-1.02238800	C	0.64208600	3.67110400	-0.28883800
H	-4.71316400	-2.76801300	-1.88865100	H	-0.31103500	5.55612000	0.09664200
H	-3.11794100	-3.22104600	-1.32710600	H	-1.28776800	4.16254000	0.50191000
O	-1.75583300	-0.04856700	0.06769600	O	1.00979600	1.31110700	-0.35262800
C	-2.84659200	-0.80438100	-2.32048800	C	0.01391700	3.48548900	-1.67777400
H	-2.57996700	0.25401800	-2.35167000	H	0.63270200	2.85807800	-2.32076400
H	-1.93588700	-1.39811700	-2.43326200	H	-0.97733600	3.02914200	-1.60465300
H	-3.50607300	-1.01662200	-3.16842500	H	-0.09555900	4.46807200	-2.14769200
C	-4.79009600	-0.19907700	-0.85453700	C	2.06672000	4.24430600	-0.44660000
H	-5.42356100	-0.24526800	-1.74716200	H	2.02357100	5.17504900	-1.02201600
H	-5.41185300	-0.44714200	0.00903700	H	2.54321300	4.46504400	0.51183800
H	-4.43668400	0.83083200	-0.73929500	H	2.69744000	3.53494600	-0.99164700
C	-1.63664700	-2.85415200	1.38238600	C	-0.78650000	1.63741700	2.21779300
H	-0.65604400	-2.38037000	1.28211700	H	-1.01717500	0.72870100	1.65285600
H	-1.65372200	-3.41783700	2.32180500	H	-0.84498400	1.40271500	3.28618300
H	-1.76730100	-3.56408400	0.56032900	H	-1.55470500	2.38303000	1.99410900
C	-2.52797900	-0.83778000	2.59755100	C	1.67860100	1.10905300	2.31406800
H	-1.52185100	-0.41564800	2.59537800	H	1.45091900	0.11131600	1.93566700
H	-3.25008700	-0.01493400	2.58393500	H	2.67833900	1.39218700	1.97036500
H	-2.66657400	-1.40044700	3.52658300	H	1.69226300	1.06273900	3.40778600

O	0.85259600	-0.36824900	-1.96698200	O	0.30333100	-0.80515100	-2.79336000
O	0.54396800	-1.70757900	-2.21778400	O	-0.02577200	0.35800100	-3.42986400
H	1.42616800	-2.10082000	-2.37059900	H	-0.47606900	0.04555700	-4.24327800
H	5.73793000	-0.41808500	-1.17965900	H	-5.84912400	-2.03678900	-1.04355300
C	5.78032200	-1.08112100	-0.31216500	C	-5.70084600	-1.22674900	-0.32589800
C	4.48306900	-1.29426400	0.41934700	C	-4.28002200	-0.77354200	-0.12963100
C	6.94764000	-1.64308800	0.01371400	C	-6.76658000	-0.70823400	0.29105400
C	3.39902400	-1.94996200	-0.45776800	C	-3.63921900	-0.23099100	-1.42005600
H	4.09229400	-0.33191500	0.78130500	H	-3.66723000	-1.61568400	0.22506100
H	4.65514000	-1.91772700	1.30718300	H	-4.24236700	-0.00119400	0.65170400
H	6.98475200	-2.30638300	0.88050700	H	-6.61369300	0.10352800	1.00583300
C	8.24412100	-1.43844000	-0.71507400	C	-8.18762200	-1.14965300	0.09041000
C	2.05342800	-2.10739200	0.25498000	C	-2.19041200	0.23223200	-1.24221300
H	3.74320200	-2.94184600	-0.78111600	H	-4.22974700	0.61746300	-1.79138800
H	3.26138100	-1.34457700	-1.36612300	H	-3.66690700	-1.00371800	-2.19961700
H	9.00912200	-1.01336400	-0.05181200	H	-8.63254200	-1.49853100	1.03194600
H	8.64603300	-2.39123900	-1.08445900	H	-8.81483300	-0.32010600	-0.26250100
H	8.12499600	-0.76535400	-1.57070900	H	-8.25857600	-1.96261500	-0.63981200
O	1.47808600	-0.90546600	0.68644000	O	-1.35391400	-0.82382900	-0.87932900
H	2.18698300	-2.70109300	1.17613100	H	-2.14779700	1.03812700	-0.48553700
H	1.34198000	-2.68670200	-0.35452700	H	-1.83816200	0.69305400	-2.18637200

TS3-4

Charge=1 Multiplicity = 2

C	0.31905200	-3.56845400	-0.56141300
C	0.04414100	-4.87864600	-0.94651800
C	-1.28703800	-5.26709500	-1.08446200
C	-2.30079700	-4.34257000	-0.83267000
C	-1.95429500	-3.04588300	-0.45224100
N	-0.65735000	-2.67981900	-0.33192900
H	-1.53889700	-6.28019600	-1.38235800
H	1.32809400	-3.19714700	-0.42052300
H	0.85806500	-5.57162800	-1.12876700
H	-3.33962900	-4.63482800	-0.93112700
H	-6.20380300	-1.11894900	0.03215000
C	-5.12364500	-1.01928400	0.07612900
C	-4.53524300	0.19572100	0.41891700
C	-4.30954100	-2.11174600	-0.22081900
C	-3.14502300	0.27570400	0.46203400
H	-5.13439700	1.07066600	0.64583300
C	-2.92399300	-1.96464500	-0.15455800
H	-4.75309500	-3.06014200	-0.50002400
N	-2.36316300	-0.77956300	0.19240400

TS3-4

Charge=1 Multiplicity = 4

C	0.31905200	-3.56845400	-0.56141300
C	0.04414100	-4.87864600	-0.94651800
C	-1.28703800	-5.26709500	-1.08446200
C	-2.30079700	-4.34257000	-0.83267000
C	-1.95429500	-3.04588300	-0.45224100
N	-0.65735000	-2.67981900	-0.33192900
H	-1.53889700	-6.28019600	-1.38235800
H	1.32809400	-3.19714700	-0.42052300
H	0.85806500	-5.57162800	-1.12876700
H	-3.33962900	-4.63482800	-0.93112700
H	-6.20380300	-1.11894900	0.03215000
C	-5.12364500	-1.01928400	0.07612900
C	-4.53524300	0.19572100	0.41891700
C	-4.30954100	-2.11174600	-0.22081900
C	-3.14502300	0.27570400	0.46203400
H	-5.13439700	1.07066600	0.64583300
C	-2.92399300	-1.96464500	-0.15455800
H	-4.75309500	-3.06014200	-0.50002400
N	-2.36316300	-0.77956300	0.19240400

H	-2.62359700	1.20159300	0.67925100	H	-2.62359700	1.20159300	0.67925100
Cu	-0.37410000	-0.81233400	0.30802900	Cu	-0.37410000	-0.81233400	0.30802900
H	-1.19557700	4.40508500	-2.75349300	H	-1.19557700	4.40508500	-2.75349300
C	-1.59954800	3.76961300	-1.95694700	C	-1.59954800	3.76961300	-1.95694700
C	-1.93541500	4.62994300	-0.72558000	C	-1.93541500	4.62994300	-0.72558000
C	-0.56330600	2.63181900	-1.68340900	C	-0.56330600	2.63181900	-1.68340900
H	-2.52318100	3.33286200	-2.35330500	H	-2.52318100	3.33286200	-2.35330500
H	-2.75598200	4.17108100	-0.16043800	H	-2.75598200	4.17108100	-0.16043800
C	-0.71525500	4.78269300	0.18186500	C	-0.71525500	4.78269300	0.18186500
H	-2.29668900	5.61284200	-1.04752200	H	-2.29668900	5.61284200	-1.04752200
N	-0.61876900	2.34251800	-0.21466600	N	-0.61876900	2.34251800	-0.21466600
C	-0.26075800	3.42322500	0.77341900	C	-0.26075800	3.42322500	0.77341900
H	-0.92852100	5.46353800	1.01382000	H	-0.92852100	5.46353800	1.01382000
H	0.10480000	5.24180100	-0.38336800	H	0.10480000	5.24180100	-0.38336800
O	0.04837000	1.15472400	0.12672400	O	0.04837000	1.15472400	0.12672400
C	1.23801300	3.47433200	1.13053200	C	1.23801300	3.47433200	1.13053200
H	1.55737100	2.57075300	1.65751100	H	1.55737100	2.57075300	1.65751100
H	1.87434100	3.60645700	0.25185200	H	1.87434100	3.60645700	0.25185200
H	1.41548000	4.32672600	1.79555500	H	1.41548000	4.32672600	1.79555500
C	-1.05846200	3.12511100	2.05784500	C	-1.05846200	3.12511100	2.05784500
H	-0.77808600	3.82760700	2.85021400	H	-0.77808600	3.82760700	2.85021400
H	-2.13674600	3.22426900	1.88921700	H	-2.13674600	3.22426900	1.88921700
H	-0.85317700	2.11165900	2.41546900	H	-0.85317700	2.11165900	2.41546900
C	0.83960400	3.02859900	-2.20093400	C	0.83960400	3.02859900	-2.20093400
H	1.59696000	2.28582400	-1.92955300	H	1.59696000	2.28582400	-1.92955300
H	0.81784100	3.08738000	-3.29492600	H	0.81784100	3.08738000	-3.29492600
H	1.16602700	4.00311200	-1.83157400	H	1.16602700	4.00311200	-1.83157400
C	-1.00854400	1.37313200	-2.44842400	C	-1.00854400	1.37313200	-2.44842400
H	-0.26599200	0.57081200	-2.39389400	H	-0.26599200	0.57081200	-2.39389400
H	-1.96475300	0.99878700	-2.07034500	H	-1.96475300	0.99878700	-2.07034500
H	-1.14119800	1.62532200	-3.50561200	H	-1.14119800	1.62532200	-3.50561200
H	1.22226100	1.00292000	-0.10033700	H	1.22226100	1.00292000	-0.10033700
O	-0.33912200	-1.17273500	2.64099400	O	-0.33912200	-1.17273500	2.64099400
O	-1.17695300	-0.47759400	3.40894800	O	-1.17695300	-0.47759400	3.40894800
H	-0.79290900	-0.53449400	4.31392900	H	-0.79290900	-0.53449400	4.31392900
H	8.48026800	-0.34232100	1.06486300	H	8.48026800	-0.34232100	1.06486300
C	8.41077600	-0.55217600	-0.00762600	C	8.41077600	-0.55217600	-0.00762600
C	6.99361500	-0.80820300	-0.43170500	C	6.99361500	-0.80820300	-0.43170500
H	9.05287100	-1.41547600	-0.22750800	H	9.05287100	-1.41547600	-0.22750800
H	8.83881000	0.30132100	-0.55025100	H	8.83881000	0.30132100	-0.55025100
C	5.92971300	-0.79677000	0.37682300	C	5.92971300	-0.79677000	0.37682300
H	6.84264300	-1.02483200	-1.49155100	H	6.84264300	-1.02483200	-1.49155100
C	4.51300700	-1.04808300	-0.05751500	C	4.51300700	-1.04808300	-0.05751500
H	6.07355200	-0.57857700	1.43729500	H	6.07355200	-0.57857700	1.43729500

C	3.59684600	0.18689300	0.15752900	C	3.59684600	0.18689300	0.15752900
H	4.08163800	-1.88332300	0.51211000	H	4.08163800	-1.88332300	0.51211000
H	4.49345400	-1.33587400	-1.11727700	H	4.49345400	-1.33587400	-1.11727700
C	2.16855000	-0.06555700	-0.25188600	C	2.16855000	-0.06555700	-0.25188600
H	3.99279100	1.03292500	-0.41834300	H	3.99279100	1.03292500	-0.41834300
H	3.62000600	0.47179700	1.21714200	H	3.62000600	0.47179700	1.21714200
O	1.48216900	-0.95310100	0.49796900	O	1.48216900	-0.95310100	0.49796900
H	2.02238900	-0.17000600	-1.34500000	H	2.02238900	-0.17000600	-1.34500000

4	Charge=1 Multiplicity = 2			4	Charge=1 Multiplicity = 4		
C	-1.85732600	2.90059400	-0.08316200	C	-1.85146700	2.94497500	-0.28831400
C	-2.32607500	4.19609000	-0.29194800	C	-2.22239200	4.24967400	-0.60715300
C	-1.39721100	5.21791300	-0.47809700	C	-1.22042000	5.18357900	-0.86354700
C	-0.03416100	4.92138100	-0.44637200	C	0.11669900	4.79151300	-0.79398200
C	0.36301200	3.60073700	-0.23595900	C	0.41711700	3.46769500	-0.47212400
N	-0.54969900	2.61908700	-0.06975600	N	-0.56657000	2.57056300	-0.23271100
H	-1.72549200	6.23993900	-0.64034500	H	-1.47214900	6.20940600	-1.11440800
H	-2.51022100	2.05271100	0.09404900	H	-2.57186200	2.16548500	-0.06594700
H	-3.39249500	4.39274000	-0.30118700	H	-3.27195200	4.51926400	-0.64913900
H	0.69662700	5.71088100	-0.57643300	H	0.90449800	5.51018600	-0.98686700
H	5.02670200	4.08323300	-0.34165300	H	5.10135700	3.57332200	-0.68341100
C	4.15864800	3.44324700	-0.21703800	C	4.18818700	3.01473000	-0.50249300
C	4.30883700	2.08460900	0.05042600	C	4.23528400	1.66243600	-0.17209300
C	2.87585400	3.97776300	-0.32733800	C	2.95035100	3.64702800	-0.61064800
C	3.16490700	1.30364500	0.19730600	C	3.03739700	0.98699700	0.05177200
H	5.28940400	1.63033800	0.14089700	H	5.17789500	1.13238000	-0.09080300
C	1.77181500	3.14149000	-0.16089100	C	1.78844300	2.91307300	-0.37153000
H	2.74314400	5.03162100	-0.54136100	H	2.89738900	4.69474500	-0.88198600
N	1.92954000	1.81898900	0.10061500	N	1.84758600	1.60032800	-0.03515800
H	3.20717100	0.23284400	0.37568500	H	3.00394900	-0.07622900	0.27280000
Cu	0.21727600	0.80708000	0.28992300	Cu	0.07247900	0.75317700	0.30184200
H	4.13531400	-3.92782400	-1.20616900	H	3.16636700	-4.38674600	-2.05039200
C	3.93889300	-2.97518900	-0.70149000	C	3.27382800	-3.47235600	-1.45568600
C	4.07207100	-3.15713900	0.82254500	C	3.71741700	-3.83256400	-0.02705600
C	2.53578200	-2.47228000	-1.17543800	C	1.91923700	-2.69544700	-1.53434000
H	4.71036600	-2.27936700	-1.04996000	H	4.05952500	-2.88227800	-1.94014800
H	4.40875300	-2.22186300	1.28683900	H	4.28704800	-3.00397600	0.41098500
C	2.74170600	-3.58355100	1.44196000	C	2.50638500	-4.14161600	0.85148800
H	4.84585500	-3.90104300	1.04136100	H	4.39642400	-4.69170100	-0.05516200
N	1.95005000	-1.74700400	0.00152900	N	1.72467300	-2.04365000	-0.19567600
C	1.64296600	-2.50071800	1.26961100	C	1.59402200	-2.90120200	1.04187100

H	2.85530800	-3.78415000	2.51339600	H	2.81803300	-4.48899200	1.84307900
H	2.41267900	-4.52573000	0.98873700	H	1.93397300	-4.96373900	0.40584400
O	0.79340600	-0.97699700	-0.41408800	O	0.60868300	-1.13368300	-0.27925400
C	0.24534400	-3.15133800	1.31495500	C	0.15446100	-3.35145500	1.36444100
H	-0.54861800	-2.39828300	1.33812300	H	-0.48337000	-2.51167900	1.65721400
H	0.06688700	-3.82371200	0.47215100	H	-0.32025000	-3.87838800	0.53232000
H	0.16478200	-3.74595500	2.23151900	H	0.18692700	-4.04588300	2.21079500
C	1.74498400	-1.48293600	2.42289000	C	2.11777200	-2.05534800	2.21757200
H	1.48776000	-1.95973300	3.37509600	H	1.99731200	-2.60005000	3.16024600
H	2.75777600	-1.07746800	2.51201300	H	3.18050700	-1.82031100	2.09550100
H	1.05159000	-0.64781900	2.27672700	H	1.56156700	-1.11655700	2.30531300
C	1.68437900	-3.64291800	-1.71909200	C	0.76466500	-3.63241400	-1.96075900
H	0.67601200	-3.32167100	-1.99513200	H	-0.20704200	-3.12487000	-1.93192700
H	2.15996800	-4.03496900	-2.62501100	H	0.92488300	-3.95494100	-2.99525700
H	1.60657400	-4.47417900	-1.01404600	H	0.70122700	-4.53388500	-1.34664200
C	2.73093800	-1.46003700	-2.31802300	C	2.05044600	-1.58372900	-2.59050100
H	1.78034600	-1.15054600	-2.75962400	H	1.10302500	-1.06700600	-2.76537100
H	3.26120800	-0.56775200	-1.97037300	H	2.80127800	-0.84665600	-2.28762500
H	3.33375200	-1.92404600	-3.10564000	H	2.37363300	-2.02558200	-3.53890400
H	0.01946300	-1.55685700	-0.63149800	O	0.14931700	0.93818700	2.62593300
O	-1.37778600	0.11862800	0.95448700	O	0.86245200	1.93744800	3.14015100
O	-1.19056200	0.79515900	2.24252800	H	0.56623500	1.99949600	4.07747500
H	-1.10531800	0.03415100	2.84428600	H	-0.26949600	-1.60704400	-0.34176900
H	-7.64245100	-0.16564600	1.69803200	H	-9.12154300	-1.21381900	-0.31380800
C	-8.06429400	-0.81883900	0.92697500	C	-8.27548200	-1.91173000	-0.25677600
C	-7.03842200	-1.20143100	-0.09955100	C	-6.97896600	-1.22082800	-0.56703000
H	-8.91156100	-0.29685100	0.46321300	H	-8.48182400	-2.71204800	-0.98001400
H	-8.47797100	-1.70747300	1.42155800	H	-8.26786500	-2.35360100	0.74516500
C	-5.76351900	-0.80299000	-0.10342400	C	-5.93146700	-1.13403900	0.25809100
H	-7.38489800	-1.85611900	-0.90189700	H	-6.90891700	-0.75428300	-1.55225200
C	-4.74485000	-1.19949400	-1.13837400	C	-4.63051500	-0.45292900	-0.06282400
H	-5.40524600	-0.15058300	0.69539700	H	-5.99516300	-1.60150700	1.24329200
C	-3.55392200	-1.97241600	-0.51142700	C	-3.42441500	-1.43481700	-0.08037800
H	-4.34978000	-0.30479600	-1.64209200	H	-4.41566100	0.32230500	0.68760200
H	-5.22167200	-1.81295000	-1.91357800	H	-4.70283600	0.04918400	-1.03725500
C	-2.58935200	-2.44345600	-1.55642400	C	-2.11033600	-0.76810200	-0.36682400
H	-3.95308100	-2.86856100	-0.01180000	H	-3.60745400	-2.20832000	-0.83684400
H	-3.02472600	-1.36307800	0.22779600	H	-3.36891800	-1.93989200	0.89340000
O	-1.38663300	-2.22454100	-1.57225000	O	-1.62112200	0.04870500	0.58816700
H	-3.02760700	-3.03665600	-2.38470100	H	-1.93058700	-0.46261300	-1.41074200
9				10			
Charge=1 Multiplicity = 2				Charge=1 Multiplicity =2			

C	1.59940400	2.65965500	-0.09326900	C	1.85371800	1.77588500	-2.26446600
C	2.63035500	3.59347600	-0.14282400	C	2.56739700	2.83038400	-2.82433800
C	3.94348600	3.12874200	-0.12680900	C	2.47251200	4.08649200	-2.22604700
C	4.17689700	1.75611300	-0.06474200	C	1.66441900	4.23982600	-1.10260000
C	3.09209000	0.87810800	-0.02026100	C	0.96650600	3.13676600	-0.60245600
N	1.81539100	1.33655700	-0.03474200	N	1.06971800	1.91356300	-1.18220800
H	4.77796000	3.82219800	-0.16028700	H	3.02028800	4.93452700	-2.62498100
H	0.55995700	2.97148100	-0.10204600	H	1.90108600	0.77841400	-2.69066100
H	2.40283500	4.65279400	-0.19012300	H	3.18067500	2.66598900	-3.70379000
H	5.19416200	1.38401000	-0.04535400	H	1.59179900	5.20598300	-0.61707600
H	5.43825200	-3.18409400	0.04869500	H	-1.53649500	5.28109100	2.73154300
C	4.49010700	-2.65654100	0.08117300	C	-1.20677100	4.35932600	2.26252300
C	3.29043300	-3.35490300	0.19851800	C	-1.63938300	3.12215100	2.73830000
C	4.46102100	-1.26527400	0.00436000	C	-0.34640800	4.39875500	1.16806400
C	2.10408300	-2.62795900	0.23230300	C	-1.19077700	1.97238000	2.09654500
H	3.26670500	-4.43716900	0.26367000	H	-2.30945900	3.04391600	3.58765000
C	3.23297000	-0.60234500	0.04820200	C	0.06458200	3.20205600	0.57474700
H	5.38772200	-0.71254800	-0.09241900	H	-0.01717700	5.35300300	0.77377600
N	2.06749200	-1.28826000	0.15815100	N	-0.35490700	1.99946200	1.04466000
H	1.14377300	-3.12541000	0.32167700	H	-1.49571500	0.98687200	2.43401400
Cu	0.48711800	-0.11233900	0.22688200	Cu	0.15946800	0.48051900	-0.12487500
H	-5.88217000	-0.15886500	-1.06460900	O	-1.61832300	-0.49466400	-0.71999500
C	-4.91311800	0.34505900	-1.13853300	H	4.36713100	-4.46196000	1.41040800
C	-3.87442100	-0.67985300	-1.63690700	C	4.31613500	-3.42967200	1.04883900
C	-4.53698600	0.98776700	0.21448900	C	3.45259100	-2.61305100	2.03065100
H	-5.04639100	1.14107200	-1.87868300	C	3.78464800	-3.39255800	-0.40027300
H	-3.88838900	-0.73245200	-2.73104600	H	5.34741200	-3.06142300	1.05103500
C	-2.42207600	-0.40786100	-1.20223600	H	4.06740000	-2.24423500	2.85942300
H	-4.14505600	-1.68188800	-1.28723400	C	2.72176000	-1.40238600	1.41180100
C	-3.59931400	0.14197500	1.10425700	H	2.69436500	-3.26059400	2.48395700
H	-5.44048900	1.21055000	0.79246800	C	2.27144600	-3.13087000	-0.53626900
H	-4.04280300	1.95149400	0.04236600	H	4.00988500	-4.33483500	-0.91156100
N	-2.39853900	-0.20772800	0.27740600	H	4.30666300	-2.61143900	-0.96547300
C	-1.83178600	0.84417100	-1.88209000	N	1.95574900	-1.87970600	0.21503500
C	-1.55881800	-1.63386200	-1.54703400	C	3.71428000	-0.30408700	0.97150000
C	-3.15311100	0.97991800	2.31165600	C	1.73805900	-0.83295800	2.44482000
C	-4.27159000	-1.15335700	1.60854800	C	1.93564600	-2.90527200	-2.02102500
O	-1.23424200	-0.14017600	0.87201500	C	1.42017100	-4.29916700	0.00739500
H	-0.81869300	1.01565400	-1.49868700	O	0.81778500	-1.30447900	-0.08927600
H	-1.76321900	0.69325700	-2.96387000	H	3.18298800	0.52536900	0.49327200
H	-2.43173100	1.73855700	-1.69339100	H	4.24484700	0.09041000	1.84489200
H	-0.52199000	-1.47513700	-1.23186800	H	4.45952000	-0.68295900	0.26661500
H	-1.93422700	-2.53440900	-1.05116800	H	1.15530500	-0.01432500	2.01897200
H	-1.56098500	-1.80057900	-2.62806700	H	1.04156100	-1.60325800	2.79151900

H	-2.51239800	0.40886300	2.98624200	H	2.29629300	-0.45472000	3.30629500
H	-2.61156800	1.87731100	1.99728300	H	0.86485500	-2.75343700	-2.17262800
H	-4.04382200	1.29389600	2.86482500	H	2.47054800	-2.03432100	-2.41520200
H	-5.10682200	-0.89872200	2.26968400	H	2.24274300	-3.78287300	-2.59851500
H	-4.66506800	-1.77019200	0.79688900	H	1.56761800	-5.18732200	-0.61625200
H	-3.55620300	-1.75260400	2.18086000	H	1.68082300	-4.56315400	1.03553000
				H	0.35800100	-4.03588600	-0.01957500
				C	-2.62204100	-0.22858700	-1.72981200
				H	-2.87248200	0.82809600	-1.59936800
				C	-3.85623700	-1.10798300	-1.56660600
				H	-4.53133600	-0.90159700	-2.40731700
				H	-3.56327500	-2.16403200	-1.66936400
				C	-4.60491200	-0.89638500	-0.23731900
				H	-3.89813400	-1.05751300	0.58967300
				H	-4.93281400	0.14993800	-0.17054500
				C	-5.79044100	-1.81142900	-0.08551100
				H	-5.57076000	-2.88135000	-0.06830800
				C	-7.06070000	-1.41117600	0.01646400
				H	-7.27501200	-0.34033100	-0.00187100
				C	-8.24836100	-2.31771800	0.16204000
				H	-8.79405200	-2.11011500	1.09205600
				H	-8.96258400	-2.16951700	-0.65870600
				H	-7.95370700	-3.37231300	0.16970000
				H	-2.17694200	-0.35343600	-2.72574600
				H	-1.34305800	-1.42613200	-0.77205700
TS 10-11				11			
Charge=1 Multiplicity = 2				Charge=1 Multiplicity =2			
C	3.07337000	1.21288800	-1.36851700	C	2.85034500	1.39657300	-1.54773000
C	4.16249500	2.02715900	-1.66567200	C	3.93011200	2.25143300	-1.74906600
C	4.13510600	3.35404400	-1.24280500	C	3.89691500	3.51313800	-1.15873900
C	3.02255000	3.82363200	-0.54582300	C	2.78952500	3.88003400	-0.39502700
C	1.96176000	2.95583400	-0.28696400	C	1.73977000	2.97528300	-0.23745900
N	2.00126900	1.66083900	-0.69718800	N	1.78513900	1.74435000	-0.81022300
H	4.96619500	4.02001600	-1.45285600	H	4.71959100	4.20856700	-1.29256500
H	3.04580500	0.17109200	-1.66315400	H	2.82381600	0.40297800	-1.98030500
H	5.00619300	1.62243300	-2.21353200	H	4.76999300	1.92973800	-2.35474400
H	2.98530100	4.85509500	-0.21616500	H	2.74651100	4.86176200	0.06159800
H	-0.94225100	5.83744500	2.02075500	H	-1.14242000	5.45723600	2.51977900
C	-0.73907500	4.85946700	1.59560600	C	-0.94258800	4.55813600	1.94525000
C	-1.68625200	3.84038400	1.67783200	C	-1.88429000	3.53216800	1.88488600
C	0.47867300	4.61638600	0.95915300	C	0.26661300	4.42283300	1.26219600

C	-1.37988400	2.60146100	1.11945700	C	-1.58360100	2.39678600	1.13648600
H	-2.64384400	3.99478000	2.16270900	H	-2.83356000	3.60320300	2.40418800
C	0.71906700	3.35184200	0.42161900	C	0.50289800	3.25852100	0.53122300
H	1.22089200	5.40281000	0.89004800	H	1.00749600	5.21229200	1.30736000
N	-0.20683700	2.36983300	0.51441300	N	-0.42134200	2.27145900	0.48226400
H	-2.06917200	1.76388600	1.14116800	H	-2.26689900	1.55949300	1.04324000
Cu	0.35254100	0.64365700	-0.28295100	Cu	0.12414600	0.68850400	-0.55803500
O	-1.40415000	-0.16001700	-0.44362600	O	-1.46834500	-0.13514600	-0.87527100
H	0.80636500	-5.07350000	1.12446300	H	3.49222200	-4.73985000	1.87639200
C	1.79448200	-4.71521600	1.43535200	C	3.36207500	-3.66000800	1.74947000
C	1.65297600	-3.50137200	2.36319200	C	1.96645600	-3.26697800	2.27738000
C	2.62105400	-4.33706200	0.20926900	C	3.57358100	-3.26710400	0.27266200
H	2.26958300	-5.53842400	1.98035100	H	4.14545700	-3.19128800	2.35518500
H	2.57068400	-3.38920800	2.95291900	H	2.00978900	-3.04776700	3.35005900
C	1.38911300	-2.14802600	1.61665800	C	1.33471700	-2.05184100	1.56645300
H	0.84690000	-3.68370700	3.08149800	H	1.27383500	-4.10831600	2.16632800
C	1.89062500	-3.29703500	-0.67587700	C	2.27636200	-3.22492700	-0.56652500
H	2.84384800	-5.21480100	-0.40761800	H	4.26775300	-3.96662200	-0.20703400
H	3.59039900	-3.93771300	0.53791300	H	4.05500300	-2.28401600	0.21159600
N	1.02763400	-2.45943500	0.20902000	N	1.19045300	-2.44589600	0.14163600
C	2.61449700	-1.21239300	1.72885100	C	2.17179300	-0.77519000	1.80680700
C	0.17766200	-1.46643500	2.27892700	C	-0.08434900	-1.83571500	2.12713200
C	2.92270800	-2.49841500	-1.49576800	C	2.60596100	-2.63584400	-1.94495200
C	0.93633000	-4.01471300	-1.65253700	C	1.71514800	-4.64991700	-0.77527900
O	0.52646200	-1.34913000	-0.50413600	O	0.69311400	-1.33457900	-0.65393800
H	2.46473500	-0.31506200	1.11815800	H	1.72932700	0.08234800	1.29068000
H	2.75847900	-0.89358300	2.76732900	H	2.18881100	-0.53856100	2.87612800
H	3.53678500	-1.70045300	1.40104000	H	3.20568700	-0.87078500	1.46778100
H	-0.02317100	-0.47121500	1.86845200	H	-0.61112600	-1.03598800	1.59647200
H	-0.72496700	-2.07116800	2.14871000	H	-0.67763300	-2.74889200	2.02114100
H	0.36609500	-1.34728200	3.35062100	H	-0.04114900	-1.57029600	3.18911400
H	2.42426400	-1.83194100	-2.20636500	H	1.72749800	-2.57785800	-2.59191100
H	3.59141600	-1.91611400	-0.85377200	H	3.04629700	-1.63753000	-1.86183800
H	3.54257700	-3.19323700	-2.07274000	H	3.34354300	-3.28159400	-2.43218800
H	1.50449900	-4.62328100	-2.36466800	H	2.44450400	-5.27755200	-1.30029800
H	0.24436900	-4.66937500	-1.11403900	H	1.47164200	-5.13578700	0.17337100
H	0.34723100	-3.28678700	-2.21801400	H	0.79868500	-4.61216200	-1.37293500
C	-2.21073200	0.04297000	-1.61051800	C	-2.44669700	0.43342600	-1.72427600
H	-2.37116800	1.12437300	-1.73336500	H	-2.68467700	1.46471400	-1.40393200
C	-3.55671800	-0.66840700	-1.48475600	C	-3.72891800	-0.40365000	-1.69868600
H	-4.09500300	-0.55128300	-2.43463400	H	-4.42716800	0.00610100	-2.44047300
H	-3.37756100	-1.74461600	-1.35772000	H	-3.48241700	-1.42238300	-2.02626100
C	-4.42877700	-0.14259600	-0.33040300	C	-4.40694300	-0.45069500	-0.31776100
H	-3.85824400	-0.24368900	0.60443400	H	-3.66635200	-0.80692900	0.41281100

H	-4.61786800	0.93065900	-0.47745100	H	-4.69247400	0.56852200	-0.01728600
C	-5.73927100	-0.87266000	-0.20788400	C	-5.62002700	-1.34065000	-0.28881300
H	-5.67183100	-1.94079900	0.00985200	H	-5.44034700	-2.39620800	-0.50475900
C	-6.94531700	-0.31799400	-0.35636100	C	-6.86803600	-0.93683400	-0.03658900
H	-7.00659600	0.75032700	-0.57622700	H	-7.04360100	0.12029300	0.17583600
C	-8.25566000	-1.04229800	-0.24389200	C	-8.08046500	-1.82246100	-0.01393700
H	-8.88058300	-0.61196500	0.55000000	H	-8.57368600	-1.79641500	0.96696900
H	-8.83364600	-0.96252500	-1.17416200	H	-8.82735800	-1.49209800	-0.74808000
H	-8.11213200	-2.10528700	-0.02366900	H	-7.82377900	-2.86349400	-0.23642600
H	-1.67850500	-0.31742300	-2.50389500	H	-2.08117200	0.49980600	-2.76247900
H	-0.64742100	-1.13869800	-0.47124900	H	-0.24793000	-1.55197100	-0.84220800
12				12			
Charge=1 Multiplicity = 1				Charge=1 Multiplicity = 3			
C	-3.24749600	1.06616200	-0.27027000	C	-3.23967900	0.97851600	-0.07725600
C	-4.42090700	1.46966400	-0.90131500	C	-4.39771200	1.45367900	-0.68641600
C	-4.93156100	0.67028900	-1.92341800	C	-4.90388700	0.75588000	-1.78248700
C	-4.25574100	-0.49505500	-2.27645300	C	-4.23793300	-0.38280800	-2.22928300
C	-3.08690200	-0.84057200	-1.59177800	C	-3.08337700	-0.80305800	-1.56263100
N	-2.60213800	-0.06079400	-0.59843500	N	-2.60451600	-0.12411000	-0.49530000
H	-5.84058400	0.95239600	-2.44583400	H	-5.80142500	1.09636500	-2.28971500
H	-2.78599500	1.65789800	0.51257000	H	-2.78601800	1.49024200	0.76405700
H	-4.91323800	2.38838900	-0.60125600	H	-4.88198700	2.34950500	-0.31299200
H	-4.63069800	-1.11812300	-3.07994700	H	-4.60773700	-0.92703800	-3.09034300
H	-2.09520800	-4.94725100	-3.63790000	H	-2.11081800	-4.73313100	-3.93937700
C	-1.82112800	-4.15738400	-2.94520700	C	-1.83315200	-4.00378800	-3.18453400
C	-0.64298000	-4.23768600	-2.20566900	C	-0.65569900	-4.15058000	-2.45395300
C	-2.65754300	-3.05394000	-2.77865600	C	-2.66457900	-2.91353100	-2.92858500
C	-0.33673200	-3.20057000	-1.32595300	C	-0.34445500	-3.19131600	-1.49159600
H	0.02622800	-5.08612100	-2.29935100	H	0.00935900	-4.99171800	-2.61691700
C	-2.28100700	-2.05177400	-1.88194200	C	-2.28451900	-1.99054800	-1.95249300
H	-3.58769100	-2.98882300	-3.33121100	H	-3.59434400	-2.79901600	-3.47378100
N	-1.12930700	-2.13263400	-1.18307800	N	-1.13415600	-2.13621300	-1.26142500
H	0.54595400	-3.19948500	-0.69555200	H	0.53663700	-3.24354700	-0.86101000
C	-1.19055300	-1.11663600	4.38309300	C	-1.01343900	-1.17501100	4.41885400
C	-0.53007900	-1.03620200	3.18816400	C	-0.39527900	-1.09868700	3.20145100
C	-2.61210000	-0.60902100	2.78243400	C	-2.50508400	-0.75425000	2.85706000
N	-2.51842300	-0.84188700	4.11275900	N	-2.35864800	-0.95403100	4.18725800
H	-0.84960600	-1.34218900	5.38216200	H	-0.63203500	-1.36579200	5.41047200
H	0.50790700	-1.19487200	2.94074600	H	0.63708000	-1.23395300	2.91954500
H	-3.54850700	-0.37807400	2.29560400	H	-3.46468600	-0.57090500	2.39621300
N	-1.42969000	-0.71555900	2.19049800	N	-1.33868600	-0.83319500	2.22844000
C	-3.61164600	-0.82505300	5.07799500	C	-3.41920100	-0.95256700	5.18880700
H	-3.72959000	-1.81172600	5.53427600	H	-3.47115200	-1.92527600	5.68523200

H	-3.41452300	-0.08645400	5.85971700	H	-3.23409900	-0.17495500	5.93484600
H	-4.53697000	-0.55901600	4.56380300	H	-4.37334300	-0.75388200	4.69743400
H	4.70949300	-0.44124400	-0.51325900	H	4.65813200	-0.36585800	-0.49748900
C	4.44455200	-1.50599500	-0.57015900	C	4.45680200	-1.44033900	-0.60801400
C	3.19292600	-1.77630700	0.28584500	C	3.22043600	-1.82419200	0.22656600
H	4.20029200	-1.70891900	-1.62533400	H	4.22858000	-1.60533700	-1.67328300
C	5.62620800	-2.34197500	-0.15780100	C	5.68472300	-2.22370500	-0.22881800
C	1.96627300	-0.97136600	-0.16331100	C	1.95658100	-1.05251100	-0.17459600
H	3.40372100	-1.53928900	1.33634400	H	3.42027000	-1.64077100	1.28985800
H	2.94488700	-2.84690800	0.25773000	H	3.02425900	-2.90161500	0.13271100
H	5.49324400	-3.42392800	-0.23120400	H	5.61953300	-3.30637700	-0.35982200
C	6.78986600	-1.86566700	0.29279000	C	6.81323200	-1.70081500	0.25817000
O	0.87301200	-1.25573500	0.65792700	O	0.87886700	-1.43801300	0.62937200
H	6.91919500	-0.78354700	0.36615900	H	6.87400200	-0.61807100	0.38897300
C	7.96647400	-2.69961100	0.71175200	C	8.03659400	-2.48073800	0.64616200
Cu	-0.80545100	-0.63842500	0.20457200	Cu	-0.80862900	-0.78788700	0.24109500
H	8.85422000	-2.46697700	0.10844500	H	8.91260800	-2.16228200	0.06528400
H	8.23998700	-2.50554600	1.75766100	H	8.28957800	-2.32473700	1.70358400
H	7.75883900	-3.77001900	0.60902700	H	7.89728700	-3.55521700	0.48632400
H	2.22822900	0.10174400	-0.14567000	H	2.16724300	0.02867700	-0.09458800
H	1.75994300	-1.21529300	-1.22758400	H	1.75903500	-1.24285900	-1.25174400
H	1.67775600	2.67335700	2.84856200	H	1.65335400	2.75564800	2.83976500
C	1.26712700	2.14745500	1.98020900	C	1.27381400	2.20875200	1.97018000
C	1.02548900	3.16536600	0.85580900	C	0.94283000	3.21344900	0.85626800
H	0.34100100	1.65593300	2.28198800	H	0.39264800	1.64228000	2.27593900
H	1.97909800	1.37644500	1.67507500	H	2.04160800	1.49933200	1.64849400
C	2.34551500	3.88020800	0.51281300	C	2.20833200	4.01392800	0.49454000
N	0.56145500	2.43322400	-0.37303900	N	0.50659200	2.45506600	-0.36443300
C	-0.07665200	4.15273400	1.29774700	C	-0.21205600	4.12643000	1.32182500
C	2.27876100	4.81562000	-0.71320600	C	2.06609200	4.93721100	-0.73435600
H	2.66439500	4.43937600	1.39924900	H	2.50030100	4.59701800	1.37489400
H	3.10829400	3.10921400	0.35493000	H	3.01870100	3.29481000	0.32966000
C	0.88849100	2.89012200	-1.77438900	C	0.78899600	2.92157000	-1.76888000
O	-0.34647600	1.53074900	-0.22557800	O	-0.30325400	1.46537500	-0.20293600
H	0.20789800	4.61563200	2.24864400	H	0.05859700	4.60978500	2.26664000
H	-0.24514000	4.95223400	0.57199600	H	-0.44669400	4.91076900	0.59753200
H	-1.01965000	3.61793100	1.44901700	H	-1.11467200	3.53043800	1.49086900
C	1.19812400	4.40168100	-1.73323500	C	1.00390300	4.44894600	-1.74076600
H	2.08139700	5.84510500	-0.39623200	H	1.80468300	5.95289300	-0.41897300
H	3.26356500	4.83396600	-1.19162900	H	3.04242800	5.01815800	-1.22363200
C	2.08788400	2.08589800	-2.31539000	C	2.02872300	2.18204200	-2.31248600
C	-0.33420800	2.64792400	-2.67168400	C	-0.42671900	2.59721100	-2.65007600
H	1.49645000	4.70666900	-2.74252900	H	1.27029200	4.76830100	-2.75454700
H	0.26214000	4.93236900	-1.52568700	H	0.03809000	4.91911300	-1.52321700

H	1.86542400	1.01575200	-2.31954700	H	1.87555400	1.09985800	-2.27851800
H	2.29551300	2.39646700	-3.34538100	H	2.19830000	2.47207700	-3.35542800
H	2.99568700	2.24364300	-1.72731300	H	2.93511200	2.41597800	-1.74772100
H	-0.54827400	1.58318100	-2.78372400	H	-0.57334100	1.52019800	-2.75239600
H	-1.22515600	3.13980300	-2.26920700	H	-1.34160400	3.03343200	-2.23686200
H	-0.13014500	3.06418200	-3.66357200	H	-0.26381400	3.01964100	-3.64693500
TS 12-13				TS 12-13			
Charge=1 Multiplicity =1				Charge=1 Multiplicity =3			
C	-2.29634100	1.69163800	1.08653900	C	-2.66913600	1.59351000	0.11029800
C	-3.39255800	2.48273800	1.41880500	C	-3.63578500	2.44321200	-0.42210800
C	-4.60725900	2.23316000	0.78246600	C	-4.34976800	2.01883700	-1.54146100
C	-4.67676300	1.21672300	-0.16645300	C	-4.07045600	0.77048700	-2.09515100
C	-3.53434700	0.46283300	-0.45223100	C	-3.08824600	-0.03035100	-1.50834900
N	-2.36119700	0.70131200	0.18414200	N	-2.41336100	0.38557800	-0.41009000
H	-5.48775400	2.82487100	1.01356600	H	-5.10876400	2.65410100	-1.98756500
H	-1.32060500	1.86224900	1.52626500	H	-2.06982400	1.87772800	0.96772800
H	-3.28951600	3.27428400	2.15334600	H	-3.81375700	3.41347000	0.02859500
H	-5.61069000	1.01711800	-0.67820800	H	-4.60170500	0.43596700	-2.97841900
H	-5.25074400	-2.31647400	-3.82241100	H	-3.30871900	-3.81600200	-4.27614400
C	-4.41921900	-2.01548000	-3.19249000	C	-2.82537300	-3.27651700	-3.46747000
C	-3.18000300	-2.64366700	-3.30206500	C	-1.71875500	-3.81718900	-2.81529000
C	-4.58320800	-0.98892600	-2.26360800	C	-3.31416700	-2.03279400	-3.06877900
C	-2.14432700	-2.21841500	-2.47152200	C	-1.13640600	-3.08972500	-1.77937400
H	-3.01362300	-3.44526800	-4.01369100	H	-1.31266900	-4.78290800	-3.09574300
C	-3.49676000	-0.62020100	-1.46566300	C	-2.67642400	-1.35797200	-2.02626100
H	-5.54082100	-0.48953600	-2.17298200	H	-4.18049300	-1.60647700	-3.56120200
N	-2.30176700	-1.23440500	-1.58086100	N	-1.60352200	-1.89302800	-1.40197000
H	-1.14987500	-2.65322700	-2.50010000	H	-0.28040100	-3.45120400	-1.21966100
C	-0.37148100	-3.47311000	2.87534800	C	-1.27146800	-1.60687500	4.30736100
C	-0.15437000	-2.91261700	1.64625700	C	-0.62895000	-1.56925900	3.10087600
C	-1.48452200	-1.58307900	2.70741400	C	-2.59155100	-0.70796600	2.79422500
N	-1.22256600	-2.61517700	3.54525500	N	-2.52151900	-1.05478800	4.09958800
H	-0.00942900	-4.38333500	3.32898800	H	-0.96350400	-1.96804200	5.27682600
H	0.44750800	-3.26076800	0.82134900	H	0.35523200	-1.91024000	2.82115800
H	-2.13131900	-0.76104400	2.97937000	H	-3.46885800	-0.25613900	2.35484300
N	-0.85509900	-1.72693800	1.54959100	N	-1.46444500	-1.00321800	2.15772100
C	-1.73544900	-2.78796600	4.89976500	C	-3.57006300	-0.88920900	5.10099700
H	-2.29411500	-3.72467600	4.97566500	H	-3.87323000	-1.86282700	5.49518200
H	-0.91228000	-2.79815300	5.61945300	H	-3.21178100	-0.26149800	5.92117000
H	-2.40296100	-1.95721500	5.13556100	H	-4.43327800	-0.40917800	4.63673200
Cu	-0.84564600	-0.59043300	-0.23284000	Cu	-0.90258100	-0.82002400	0.17758700
H	1.51716700	5.08797500	-1.10496800	H	1.88989100	4.52048000	-2.17304300
C	0.85256200	4.43731100	-0.52495500	C	1.05491000	4.12099500	-1.58556300

C	1.16368300	4.59021200	0.97303700	C	1.04025800	4.78544400	-0.19957200
C	1.01180600	2.98077100	-1.06990700	C	1.19282100	2.56267100	-1.54950800
H	-0.16644500	4.78955300	-0.72037400	H	0.14210500	4.39505900	-2.12667600
H	0.27364300	4.35096800	1.56848100	H	0.02444900	4.77007400	0.21420100
C	2.31392800	3.67197300	1.38090100	C	1.99156800	4.06010600	0.75019200
H	1.41045300	5.63424600	1.19545300	H	1.32099200	5.84082700	-0.29174600
N	0.95967100	2.04724200	0.10152400	N	0.79647000	2.10840300	-0.18244800
C	1.93754300	2.17542700	1.23727500	C	1.52741000	2.60818900	1.02931500
H	2.61138400	3.85040000	2.42058500	H	2.07137500	4.58726600	1.70798200
H	3.19556800	3.89961800	0.76911300	H	3.00067700	4.05712700	0.31938700
O	0.72783900	0.74390400	-0.25264200	O	0.59131200	0.73236100	-0.11378900
C	3.20943100	1.32838100	1.04584500	C	2.73251400	1.73853200	1.43769700
H	2.98401200	0.25878500	1.04468200	H	2.41891400	0.73695200	1.74486800
H	3.73579800	1.57647700	0.12099700	H	3.46477100	1.64163700	0.63188500
H	3.89526200	1.52155900	1.87803000	H	3.23922400	2.20506400	2.29000500
C	1.22226400	1.69491900	2.51507900	C	0.51009300	2.60679600	2.18828900
H	1.93042200	1.65858400	3.34986000	H	0.99485700	2.90934100	3.12327100
H	0.41162600	2.37549500	2.79922600	H	-0.31014600	3.30659800	1.99164800
H	0.81092900	0.69035900	2.37798000	H	0.09235900	1.60594200	2.33448000
C	2.31589100	2.83426400	-1.88900300	C	2.61900900	2.12899000	-1.96338300
H	2.48357100	1.79478700	-2.19105200	H	2.75575900	1.04802000	-1.85478700
H	2.23986100	3.43226400	-2.80392500	H	2.78687400	2.37653500	-3.01780800
H	3.19692700	3.18340300	-1.34457200	H	3.39597100	2.63517000	-1.38440000
C	-0.17277400	2.66663500	-1.99896700	C	0.20036300	1.96042700	-2.55992300
H	-0.06717000	1.69529000	-2.48919800	H	0.31227400	0.87641600	-2.64858000
H	-1.11682300	2.68001000	-1.44666400	H	-0.83017900	2.18594300	-2.26674800
H	-0.22431800	3.43419700	-2.77828200	H	0.37832300	2.40166800	-3.54660900
H	1.53348500	0.05037300	-0.88817800	H	1.48544100	-0.04855300	-0.23694800
C	1.60610200	-1.19170700	-1.51379900	C	1.68920600	-1.48342900	-0.31858000
H	1.64262300	-0.83426200	-2.56234500	H	1.50173600	-1.55374800	-1.40896500
O	0.45077900	-1.69383400	-1.13086900	O	0.65116700	-1.84920400	0.46491800
C	2.87442900	-1.89406800	-1.04517400	C	3.03427900	-2.03533700	0.10389300
H	2.92542200	-1.88936200	0.05121400	H	3.23430500	-1.74736100	1.14387100
H	2.78320400	-2.95251700	-1.33722100	H	2.97150100	-3.13644900	0.10531500
C	4.16644900	-1.31242000	-1.64641000	C	4.20157700	-1.59293900	-0.79873900
H	4.06266900	-1.29911300	-2.74273000	H	3.94971600	-1.83812000	-1.84297000
H	4.28995900	-0.26797100	-1.33354400	H	4.31420100	-0.50219300	-0.75343100
C	5.39054200	-2.10171500	-1.26629300	C	5.50291800	-2.25087200	-0.42629800
H	5.40317700	-3.14597900	-1.58639500	H	5.52372600	-3.34087500	-0.49572500
C	6.43053700	-1.62420100	-0.57755500	C	6.60046400	-1.60882700	-0.01747100
H	6.41363800	-0.57860800	-0.26195000	H	6.57414700	-0.51906000	0.05131000
C	7.65429400	-2.40697200	-0.19747800	C	7.89945500	-2.26152400	0.35827200
H	8.56092700	-1.95673500	-0.62313500	H	8.72089200	-1.90661000	-0.27834200
H	7.79500100	-2.42243600	0.89168200	H	8.18022400	-2.02228400	1.39276100

H	7.59528800	-3.44306300	-0.54698800	H	7.84523900	-3.35126400	0.26481700
13				13			
Charge=1 Multiplicity = 1				Charge=1 Multiplicity = 3			
C	-3.06087700	1.88644800	-0.95186400	C	-2.89715100	1.13338800	-0.29582400
C	-3.74470100	2.59633800	-1.93234000	C	-3.99296500	1.65607900	-0.97846700
C	-4.07704300	1.94458000	-3.12094200	C	-4.57330900	0.89109100	-1.98866600
C	-3.70749200	0.61273200	-3.28092600	C	-4.03876100	-0.36073100	-2.28785700
C	-3.02600000	-0.04055300	-2.24908500	C	-2.94021000	-0.82413200	-1.56024800
N	-2.71224400	0.59319600	-1.08809900	N	-2.39387500	-0.07780200	-0.57060000
H	-4.60524800	2.46616300	-3.91308900	H	-5.42635700	1.26553000	-2.54616700
H	-2.77140400	2.35475500	-0.01807100	H	-2.38923600	1.69447400	0.47993400
H	-4.00923500	3.63505500	-1.76431300	H	-4.37064900	2.64080800	-0.72581900
H	-3.92627800	0.09511900	-4.20802700	H	-4.46687900	-0.95831700	-3.08394600
H	-2.96853700	-4.38353400	-4.00021300	H	-2.35182000	-5.04616800	-3.52468700
C	-2.59261200	-3.66440600	-3.27905200	C	-2.01085300	-4.28132200	-2.83372200
C	-1.62806800	-4.03097500	-2.33892900	C	-0.86066600	-4.47528500	-2.07122900
C	-3.07322400	-2.35886300	-3.27199600	C	-2.72902600	-3.09392500	-2.69788100
C	-1.19247700	-3.07490400	-1.42877400	C	-0.46483000	-3.46620800	-1.19527800
H	-1.21932600	-5.03562900	-2.30998300	H	-0.27918800	-5.38762700	-2.14634200
C	-2.57743100	-1.44789500	-2.33300900	C	-2.27012500	-2.12489500	-1.80300000
H	-3.84057700	-2.05891600	-3.97677600	H	-3.63199500	-2.93604800	-3.27597700
N	-1.64581200	-1.80850900	-1.41167100	N	-1.15007900	-2.32243400	-1.07294900
H	-0.44652700	-3.31913900	-0.67816600	H	0.41221300	-3.55208400	-0.56373100
C	-1.24361800	-2.24478900	3.81975500	C	-1.12495800	-0.92624100	4.47067900
C	-0.70198500	-1.73594300	2.67034400	C	-0.44831600	-0.97949600	3.28365400
C	-2.84429900	-1.49517700	2.51002300	C	-2.52260100	-0.58003000	2.80701000
N	-2.60993100	-2.08645600	3.70665900	N	-2.44633600	-0.67178100	4.15420600
H	-0.79425000	-2.69617500	4.69133700	H	-0.79796200	-1.04493400	5.49249500
H	0.33427000	-1.67814500	2.37052300	H	0.59275300	-1.17193200	3.07780700
H	-3.83707600	-1.24876800	2.16263100	H	-3.44890400	-0.39016400	2.28462600
N	-1.71392900	-1.26762400	1.85161100	N	-1.33311800	-0.76078800	2.24563200
C	-3.61228900	-2.47533200	4.69243500	C	-3.55030900	-0.53584800	5.09891600
H	-3.56021800	-3.55106000	4.88105700	H	-3.66696300	-1.45624600	5.67710900
H	-3.45290200	-1.93459400	5.62932000	H	-3.36408100	0.29918800	5.77950900
H	-4.60319800	-2.23090200	4.30595900	H	-4.47139100	-0.34522400	4.54536100
Cu	-1.52468100	-0.46637100	0.08616600	Cu	-0.72958600	-0.85161100	0.27571600
H	1.92350600	4.57449700	-1.11125700	H	1.21233600	4.66610800	-2.68587900
C	0.95032000	4.12432500	-0.88213000	C	0.40934500	4.21850800	-2.08864000
C	0.34495900	4.81212800	0.35289100	C	0.19717200	5.04350300	-0.80796900
C	1.16021100	2.58158600	-0.72054900	C	0.77922300	2.71962900	-1.83494100
H	0.31160000	4.31487000	-1.75141400	H	-0.49566200	4.27053600	-2.70410000
H	-0.74805500	4.72787000	0.33269200	H	-0.83704500	4.93624200	-0.45938400
C	0.88400600	4.17939700	1.63465000	C	1.15695500	4.58794000	0.28944900

H	0.57425000	5.88352300	0.32996500	H	0.34218200	6.10788100	-1.02433900
N	0.26254200	2.14364600	0.38975400	N	0.31057500	2.38873100	-0.45365300
C	0.45027300	2.69638400	1.77336600	C	0.88120200	3.12633500	0.72811400
H	0.53572400	4.72338200	2.52035200	H	1.08012300	5.23243500	1.17281900
H	1.97906200	4.25449100	1.64182200	H	2.18924600	4.68336500	-0.06947200
O	0.18929200	0.70559000	0.45464800	O	0.40235400	0.97709200	-0.22262400
C	1.47087400	1.93541500	2.64762000	C	2.16631700	2.50613700	1.31673000
H	1.12565600	0.92547800	2.88873900	H	1.98059500	1.52143900	1.75690200
H	2.45714900	1.86589700	2.18095500	H	2.96590300	2.41130800	0.57668000
H	1.59418600	2.47216200	3.59465700	H	2.53911400	3.15615900	2.11590900
C	-0.92637200	2.61781700	2.46087700	C	-0.21017200	3.10853800	1.81589700
H	-0.85390900	2.94442100	3.50456400	H	0.15117700	3.59078300	2.73114900
H	-1.65426000	3.26066200	1.95437200	H	-1.10501800	3.64471300	1.48064400
H	-1.30170800	1.59023800	2.44982600	H	-0.48932200	2.08017500	2.06688700
C	2.65818300	2.25277900	-0.50989000	C	2.28749600	2.47476100	-2.08006300
H	2.80996400	1.18772700	-0.30100400	H	2.58470600	1.45129200	-1.81972200
H	3.21570300	2.48578000	-1.42396400	H	2.51203000	2.61142400	-3.14378600
H	3.10653600	2.83247600	0.30119700	H	2.92210200	3.16938400	-1.52410000
C	0.69752500	1.88659000	-2.01368900	C	-0.01443900	1.84912800	-2.82606000
H	0.89425700	0.81101500	-1.99851800	H	0.27338400	0.79557600	-2.77148800
H	-0.37375100	2.04156300	-2.16993300	H	-1.08858600	1.93189000	-2.63109400
H	1.23481200	2.31742900	-2.86569300	H	0.17557100	2.19793600	-3.84684600
C	3.38683500	-1.70140800	1.29984800	C	1.97305000	-1.33511700	-0.08914600
H	3.41310400	-2.70054900	1.78294200	H	1.74022600	-1.41761100	-1.16381000
O	2.31253500	-1.13633000	1.16621800	O	0.95322600	-1.51881400	0.76701200
C	4.71649100	-1.17533000	0.85003000	C	3.32250800	-1.83874700	0.34498200
H	4.59416100	-0.19544300	0.38046900	H	3.51553300	-1.51018100	1.37474700
H	5.33733500	-1.04759000	1.75054600	H	3.32365800	-2.94469100	0.38484100
C	5.43326900	-2.16925200	-0.10406900	C	4.46716500	-1.36961000	-0.57528900
H	5.49356500	-3.14968400	0.39169400	H	4.22971500	-1.66921700	-1.60873900
H	4.82850800	-2.30686500	-1.00859000	H	4.51232400	-0.27271600	-0.57254100
C	6.81234000	-1.69504900	-0.47541300	C	5.80372700	-1.93664100	-0.18051100
H	7.52126700	-1.59389100	0.34874000	H	5.88578400	-3.02585800	-0.20150300
C	7.20544200	-1.39810300	-1.71676700	C	6.86465600	-1.21748700	0.19539300
H	6.48701000	-1.50375400	-2.53247400	H	6.77804300	-0.12886100	0.21621300
C	8.57870100	-0.93269200	-2.10375200	C	8.19845100	-1.77977600	0.59517300
H	9.04242500	-1.62540500	-2.81816100	H	8.99859300	-1.40922100	-0.05950300
H	8.53939400	0.04686300	-2.59822700	H	8.46684900	-1.47932100	1.61694900
H	9.23853000	-0.84950800	-1.23411700	H	8.20453100	-2.87399400	0.55097700
H	1.06559600	0.33394300	0.69213200	H	1.34412100	0.66351500	-0.20516300
12' Charge=1 Multiplicity = 1				12' Charge=1 Multiplicity = 3			
C	2.64183000	-0.58419900	-2.12633500	C	2.09290700	-1.15044500	-2.38023700

C	3.87937700	-1.00084000	-2.61345000	C	3.05842300	-1.96911500	-2.96361000
C	4.53123000	-2.04957900	-1.96676500	C	3.54584800	-3.05065300	-2.23189700
C	3.93270500	-2.64943300	-0.85881200	C	3.06300200	-3.28253600	-0.94343500
C	2.68565300	-2.18759300	-0.43546100	C	2.09038200	-2.42641600	-0.42565900
N	2.06173900	-1.17686000	-1.07736700	N	1.61684100	-1.39202500	-1.15326200
H	5.50007300	-2.39555100	-2.31353800	H	4.30210600	-3.70608100	-2.65278800
H	2.08520500	0.24643600	-2.54887100	H	1.68009300	-0.26878500	-2.86098900
H	4.31846100	-0.50648500	-3.47303200	H	3.42084500	-1.75349700	-3.96271400
H	4.43640400	-3.45496900	-0.33714000	H	3.44716900	-4.11111800	-0.35997100
H	1.88108700	-5.03728100	3.20239300	H	1.50805700	-4.25766900	3.85363500
C	1.56305900	-4.20802300	2.57816000	C	1.24934400	-3.50023900	3.12023600
C	0.35950100	-3.55072700	2.82727500	C	0.32553500	-2.50193500	3.42476200
C	2.35503700	-3.79333300	1.50961100	C	1.84326700	-3.51662600	1.85971100
C	-0.00481600	-2.49803200	1.99347400	C	0.02424800	-1.55763300	2.44812800
H	-0.28885800	-3.84498200	3.64519300	H	-0.15565900	-2.45185100	4.39525700
C	1.93076200	-2.72309000	0.72021200	C	1.50155000	-2.53191200	0.93128200
H	3.28737700	-4.30158100	1.29366100	H	2.56387700	-4.28569100	1.60809200
N	0.76202600	-2.08485300	0.97620100	N	0.59680200	-1.56766800	1.23471700
H	-0.94041000	-1.96401100	2.11699600	H	-0.69485100	-0.76476100	2.62005400
Cu	0.30755800	-0.57378500	-0.26603400	Cu	0.24166600	-0.24166500	-0.23614100
O	0.40025100	0.96825400	-1.20160300	O	0.43168200	1.07281800	-1.49520900
C	-0.22924100	2.13066600	-0.77385200	C	0.33439500	2.41636400	-1.08718200
C	0.55834700	2.90221600	0.28991900	C	1.36904400	2.82157300	-0.02852600
H	-0.03539400	3.76390800	0.62532200	H	1.17382300	3.85489400	0.28890000
H	0.69768900	2.25557500	1.16970200	H	1.21943400	2.19660200	0.86904100
C	1.92991800	3.38989100	-0.21395000	C	2.82672700	2.69921700	-0.50657100
H	2.48260700	2.51511600	-0.58662600	H	2.97871400	1.67883600	-0.88837900
H	1.78313500	4.05684000	-1.07427300	H	2.98327000	3.37466200	-1.35825800
C	2.73156800	4.09559200	0.84521100	C	3.83162000	2.99891200	0.57251500
H	2.98664800	3.50358500	1.72783300	H	3.79645500	2.35079100	1.45264300
C	3.13345800	5.36840300	0.78631900	C	4.73236200	3.98477700	0.53926400
H	2.87506400	5.95743000	-0.09623900	H	4.76414700	4.63391200	-0.33823200
C	3.93003600	6.07937400	1.84187300	C	5.73007000	4.28859600	1.61963500
H	4.88502100	6.44383100	1.44038600	H	6.75893600	4.22306000	1.24113800
H	3.39335500	6.96071800	2.21755500	H	5.60323700	5.31038400	2.00153500
H	4.14755100	5.42586700	2.69344300	H	5.63478200	3.59718000	2.46391500
H	-5.56341200	1.78566300	-1.18918700	H	-5.97011100	1.10630400	-1.56248400
C	-5.27963000	0.99525600	-0.48700400	C	-5.54634900	0.58382600	-0.69901900
C	-4.28727300	1.58143300	0.53906700	C	-4.86237100	1.62189100	0.21326300
C	-4.71432400	-0.21954400	-1.25086600	C	-4.58810100	-0.52921700	-1.16699700
H	-6.20581400	0.68996500	0.01099600	H	-6.39331000	0.12023700	-0.18289900
H	-4.82686900	2.01031700	1.39026200	H	-5.58595700	2.04151400	0.92023200
C	-3.26476100	0.57058000	1.08481400	C	-3.67324400	1.08511100	1.03282300
H	-3.72692100	2.40867400	0.08799500	H	-4.50261300	2.46709300	-0.38348300

C	-3.18067100	-0.22142800	-1.44995300	C	-3.10246400	-0.11828500	-1.26469100
H	-5.16482100	-0.27587200	-2.24787500	H	-4.88961800	-0.89461200	-2.15440900
H	-4.99619800	-1.14961400	-0.74700000	H	-4.65470900	-1.39229100	-0.49410600
N	-2.51223700	0.01852500	-0.10312200	N	-2.70461100	0.43417100	0.08083800
C	-3.93794500	-0.58953600	1.85776100	C	-4.11446100	0.04606500	2.08464200
C	-2.29511400	1.27985600	2.04285300	C	-2.96175000	2.25866400	1.72688000
C	-2.74803400	-1.59308700	-1.99016100	C	-2.26672300	-1.36870900	-1.57943200
C	-2.76275700	0.87253600	-2.45223700	C	-2.85837900	0.94600300	-2.35507700
O	-1.49560800	-0.73886600	0.18555800	O	-1.50099200	0.28454100	0.54520600
H	-3.18607900	-1.29942600	2.21540200	H	-3.24428000	-0.37004900	2.60142300
H	-4.45932500	-0.18332300	2.73054100	H	-4.74877400	0.53518700	2.83103800
H	-4.66575500	-1.13934000	1.25957100	H	-4.68374900	-0.77843600	1.64779600
H	-1.49022100	0.61622900	2.36971000	H	-2.14376800	1.91815100	2.36448900
H	-1.85371300	2.17088100	1.59216600	H	-2.55888100	2.96442900	0.99406300
H	-2.84854500	1.59539700	2.93252600	H	-3.68646900	2.79027300	2.35133100
H	-1.68543800	-1.61552600	-2.24500900	H	-1.24216800	-1.11364800	-1.86036900
H	-2.95161200	-2.39295600	-1.27203400	H	-2.25758300	-2.07394500	-0.74206600
H	-3.31348300	-1.79933900	-2.90424900	H	-2.71373100	-1.87483700	-2.44045000
H	-3.22880800	0.66012900	-3.42045000	H	-3.14337300	0.52553800	-3.32604400
H	-3.08558200	1.86792900	-2.13583700	H	-3.45154100	1.84957500	-2.19587100
H	-1.67869800	0.87920900	-2.58434800	H	-1.79817000	1.20986400	-2.38867700
H	-1.25222400	1.89652800	-0.40359800	H	-0.67516100	2.64846800	-0.70298100
H	-0.39601400	2.77285600	-1.65520500	H	0.47318200	3.04470200	-1.98219300
TS 12'-13'				TS 12'-13'			
Charge=1 Multiplicity =1				Charge=1 Multiplicity =3			
C	0.74406300	-3.57911100	1.02685700	C	3.18432100	-1.17940100	-1.43618800
C	1.33501900	-4.83697400	1.12861900	C	4.33252400	-1.95605600	-1.57231500
C	2.62028200	-5.01029400	0.61881500	C	4.39912300	-3.17332700	-0.89698500
C	3.27461000	-3.92944800	0.02739800	C	3.32090800	-3.58270500	-0.11190900
C	2.62157500	-2.69787900	-0.03500300	C	2.20133200	-2.75657400	-0.01868600
N	1.37585000	-2.54342300	0.46432800	N	2.15491400	-1.57217500	-0.67197400
H	3.11266100	-5.97608200	0.67748600	H	5.27830200	-3.80446500	-0.98188700
H	-0.25687900	-3.36554500	1.38880100	H	3.05270700	-0.22674900	-1.93695800
H	0.79570100	-5.65459200	1.59416300	H	5.14867400	-1.60931200	-2.19638700
H	4.27330800	-4.05381700	-0.37436200	H	3.35522900	-4.53344900	0.40696600
H	5.90160100	-0.11642600	-2.17332500	H	-0.48827700	-5.22812400	2.92307900
C	4.91682400	-0.18343600	-1.72132100	C	-0.36091200	-4.36582100	2.27596200
C	4.08917100	0.93453100	-1.64763500	C	-1.38483800	-3.43407400	2.12242400
C	4.46806800	-1.39616300	-1.20108800	C	0.83852400	-4.17972400	1.58902000
C	2.83561100	0.79544300	-1.05800200	C	-1.17624100	-2.34113900	1.28429800
H	4.40187000	1.89810900	-2.03484200	H	-2.33155900	-3.54313200	2.63997400
C	3.19850400	-1.46545400	-0.62615400	C	0.98220500	-3.06535200	0.76369800
H	5.10303500	-2.27305900	-1.24485600	H	1.64833400	-4.89042700	1.70389200

N	2.39586400	-0.37228500	-0.56694600	N	-0.02354700	-2.16515500	0.61916000
H	2.15122100	1.63136100	-0.95070500	H	-1.93252400	-1.57939000	1.11399200
Cu	0.60196500	-0.70719300	0.21779800	Cu	0.44617300	-0.58386600	-0.48711100
O	-1.07174700	-1.32625500	0.83387200	O	0.94377000	0.77938000	-1.65432600
C	-2.09098400	-0.50181500	0.94552200	C	0.57283100	2.00799600	-1.22890900
C	-3.23874600	-0.64073700	-0.03452200	C	1.29981300	2.61842800	-0.04113100
H	-3.90538700	0.22709100	0.04124700	H	0.76816100	3.51998600	0.28549400
H	-2.84092000	-0.66742100	-1.05682700	H	1.28880300	1.91646600	0.80544800
C	-4.05860200	-1.93475400	0.22777500	C	2.76920000	2.99267900	-0.37872300
H	-3.36204400	-2.78312300	0.17247500	H	3.28387800	2.07794000	-0.70685700
H	-4.45717300	-1.91319800	1.25002700	H	2.77956200	3.68427400	-1.23025600
C	-5.17877400	-2.10713300	-0.75873400	C	3.48415300	3.60589200	0.79229500
H	-4.88303700	-2.22584600	-1.80349500	H	3.60161100	2.96950400	1.67250100
C	-6.47894200	-2.11214200	-0.44873300	C	3.95839100	4.85526000	0.82971300
H	-6.76779400	-1.99123800	0.59748400	H	3.83506000	5.48734800	-0.05202900
C	-7.60434700	-2.28360700	-1.42679100	C	4.66804400	5.48062600	1.99478500
H	-8.21087500	-3.16531200	-1.18112300	H	5.68024500	5.80153700	1.71548900
H	-8.28407200	-1.42137400	-1.40323500	H	4.14096500	6.37920700	2.34190900
H	-7.23640700	-2.39930900	-2.45159800	H	4.75139900	4.78741400	2.83841900
H	-1.23388400	5.57746500	1.39501400	H	-5.40371000	2.19932100	-1.47476100
C	-0.56465500	5.17947200	0.62505700	C	-5.14773900	1.54165800	-0.63729100
C	-1.38439300	4.29421000	-0.33728700	C	-4.14525100	2.26919100	0.28200600
C	0.60856500	4.41963000	1.27747100	C	-4.59753700	0.20050000	-1.16011200
H	-0.16617200	6.05036500	0.09402800	H	-6.08649700	1.35337200	-0.10548900
H	-1.81492200	4.90522900	-1.13861500	H	-4.68089700	2.86461600	1.03038100
C	-0.57505100	3.14832000	-0.98634500	C	-3.17125100	1.32633000	1.02345500
H	-2.23745800	3.85268500	0.18985100	H	-3.55378800	2.98639700	-0.29762600
C	0.35774000	2.91094500	1.45928400	C	-3.06415000	0.16681000	-1.31833500
H	0.83848200	4.84346700	2.26102200	H	-5.04046600	-0.04143000	-2.13238700
H	1.51834800	4.54421000	0.67951600	H	-4.88785800	-0.61531300	-0.48846600
N	0.11587200	2.32657700	0.09272700	N	-2.47608200	0.37771400	0.05078400
C	0.50671800	3.71315100	-1.93205900	C	-3.93153800	0.45129100	2.04388100
C	-1.52173100	2.27240000	-1.81816100	C	-2.15266300	2.17635700	1.79667800
C	1.62506100	2.24417300	2.02227900	C	-2.64941900	-1.23926100	-1.78762600
C	-0.80886300	2.66041200	2.44009900	C	-2.59669700	1.19019800	-2.37776800
O	-0.31248200	1.01425800	0.17993900	O	-1.08179200	0.61130800	-0.00566900
H	1.02312700	2.90134000	-2.45565500	H	-3.23060700	-0.17138500	2.61101700
H	0.04058700	4.35082700	-2.69119600	H	-4.46686100	1.08672900	2.75836600
H	1.25379400	4.31363600	-1.40725500	H	-4.66384100	-0.20576900	1.56868300
H	-0.99821000	1.43681400	-2.29114700	H	-1.43626900	1.55924900	2.34483500
H	-2.34939900	1.87436300	-1.22565200	H	-1.59751100	2.85494400	1.14356400
H	-1.95261000	2.89009800	-2.61244700	H	-2.69784700	2.78855900	2.52257800
H	1.52646900	1.15360600	2.01008400	H	-1.55937100	-1.35106800	-1.78051500
H	2.50862000	2.51578600	1.43565700	H	-3.07731000	-2.01542200	-1.14490200

H	1.79498900	2.55394900	3.05828400	H	-2.98781900	-1.41789600	-2.81321100
H	-0.59872200	3.17634400	3.38267900	H	-3.18226900	1.04661200	-3.29225700
H	-1.76758800	3.02987700	2.06845400	H	-2.73050300	2.22753300	-2.06206600
H	-0.91677000	1.59688200	2.67028400	H	-1.54587800	1.04225800	-2.63894300
H	-1.40719500	0.69234800	0.58715800	H	-0.65245000	1.55581500	-0.60888200
H	-2.37288600	-0.24346300	1.98118300	H	0.40055800	2.70947300	-2.05572800
13'				13'			
Charge=1 Multiplicity = 1				Charge=1 Multiplicity = 3			
C	1.42380500	0.46190000	2.54229500	C	3.14759900	-1.06535800	-1.60212800
C	2.16125600	1.19964000	3.46144700	C	4.32607400	-1.79501400	-1.73938200
C	2.45859200	2.52851700	3.16142400	C	4.48669600	-2.95346900	-0.98107800
C	2.00123800	3.06429000	1.96079100	C	3.46677100	-3.35626000	-0.11863900
C	1.25970800	2.26497000	1.08627400	C	2.31034100	-2.58140600	-0.03229700
N	0.97878400	0.96673200	1.37708000	N	2.17510400	-1.45083600	-0.76370900
H	3.03724100	3.13819700	3.84823800	H	5.39366700	-3.54461100	-1.06131300
H	1.16169000	-0.57217300	2.74200900	H	2.94284700	-0.15749800	-2.15854400
H	2.48911300	0.73999200	4.38766400	H	5.09406200	-1.45689100	-2.42615600
H	2.23475000	4.09059400	1.70253300	H	3.57365300	-4.26304100	0.46494200
H	0.08818100	5.51549000	-2.08007500	H	-0.13905500	-4.99909100	3.15179900
C	0.14147500	4.46947000	-1.79477600	C	-0.08028400	-4.17170900	2.45142800
C	-0.32217600	3.47153200	-2.65123600	C	-1.15875400	-3.30686100	2.27882700
C	0.66915200	4.10599500	-0.55857800	C	1.08305700	-3.96472200	1.71130300
C	-0.23985400	2.14786800	-2.23081600	C	-1.03708300	-2.25625600	1.37285700
H	-0.73970200	3.70845600	-3.62396000	H	-2.08200200	-3.43585500	2.83292400
C	0.72509000	2.75385500	-0.20823000	C	1.14009500	-2.89575400	0.81787500
H	1.01203500	4.87003900	0.12941800	H	1.93262000	-4.62560200	1.83587800
N	0.27249500	1.78577800	-1.04347700	N	0.08372000	-2.05607600	0.66005700
H	-0.59060100	1.33743800	-2.86191600	H	-1.84227600	-1.54995200	1.18294300
Cu	0.19651000	-0.00188400	-0.14730100	Cu	0.43944900	-0.51681900	-0.53956600
O	0.80754800	-1.74856600	-0.76627800	O	0.84430700	0.78088600	-1.79330300
C	1.82117700	-2.34627300	-1.14054100	C	0.66679600	2.08503300	-1.49579700
C	3.17436600	-1.73814700	-1.29005300	C	1.29596400	2.67248000	-0.25669000
H	3.55809700	-1.99086100	-2.28785100	H	0.84024900	3.64736500	-0.04345300
H	3.09936800	-0.64806500	-1.21079200	H	1.08700100	2.03127100	0.61418300
C	4.17008800	-2.30192500	-0.23027700	C	2.83707800	2.86608100	-0.37513700
H	3.78634900	-2.05077600	0.76887900	H	3.28646900	1.88536400	-0.59172500
H	4.19644400	-3.39640100	-0.29720100	H	3.05073300	3.50871400	-1.23809100
C	5.55511500	-1.74331500	-0.41458600	C	3.44436600	3.45261900	0.86857900
H	5.65753100	-0.66332200	-0.29355200	H	3.35721000	2.85029700	1.77635500
C	6.63270000	-2.47425300	-0.71318700	C	4.04852400	4.64264200	0.93957600
H	6.51718800	-3.55369400	-0.83075000	H	4.13056400	5.24190400	0.03038800
C	8.02161100	-1.93765600	-0.89706900	C	4.64459100	5.24337600	2.17928000
H	8.71666500	-2.39317500	-0.17989300	H	5.71677800	5.44038700	2.04782400
H	8.40532100	-2.17488900	-1.89787100	H	4.17717600	6.20861800	2.41522000

H	8.05872900	-0.85144200	-0.76534000	H	4.52372500	4.58604800	3.04684100
H	-5.76317000	-2.90097000	0.88458500	H	-5.60802400	1.96386000	-1.41197800
C	-5.56884700	-1.84087500	0.68841100	C	-5.30163200	1.34152000	-0.56459100
C	-5.07483600	-1.68368000	-0.76599400	C	-4.29568200	2.13188200	0.29732500
C	-4.56617700	-1.28086000	1.71827700	C	-4.72409300	0.00321100	-1.06654300
H	-6.52908400	-1.33111200	0.82021200	H	-6.21481500	1.13893800	0.00488900
H	-5.92788900	-1.55599600	-1.44227500	H	-4.82752900	2.73356800	1.04317400
C	-4.10763500	-0.49593700	-0.97536200	C	-3.27013300	1.24567200	1.03901900
H	-4.57513200	-2.60244600	-1.09589600	H	-3.74835800	2.85024400	-0.32297900
C	-3.09639100	-1.35434300	1.26567900	C	-3.19600600	0.01319000	-1.26953800
H	-4.65635600	-1.81443600	2.67120000	H	-5.18553000	-0.27953900	-2.01896800
H	-4.79484600	-0.23224000	1.93752500	H	-4.96853800	-0.80302700	-0.36566600
N	-2.97327900	-0.50787700	0.03664100	N	-2.58288900	0.26710400	0.08371900
C	-4.84277300	0.84784100	-0.78316600	C	-3.96844700	0.38773900	2.11523000
C	-3.57352800	-0.53884300	-2.41540300	C	-2.24960300	2.15142700	1.74510400
C	-2.19086100	-0.70670900	2.32721400	C	-2.73954800	-1.38698900	-1.71544400
C	-2.65552400	-2.82842900	1.07553800	C	-2.78883900	1.03019300	-2.36093400
O	-1.69303000	-0.76759800	-0.58187500	O	-1.18182000	0.59843200	-0.07691600
H	-4.14861000	1.68001900	-0.93659800	H	-3.22995900	-0.18612700	2.68577900
H	-5.66327200	0.93936200	-1.50444800	H	-4.50653600	1.03328900	2.81825600
H	-5.26605400	0.94975600	0.21907500	H	-4.68858700	-0.31477900	1.68882100
H	-2.89198500	0.29149200	-2.61779000	H	-1.49212700	1.57533500	2.28308400
H	-3.05841300	-1.47657400	-2.64925300	H	-1.74259200	2.83220400	1.05462000
H	-4.42223400	-0.45549400	-3.10170700	H	-2.78636000	2.76700000	2.47404200
H	-1.18910300	-0.56370700	1.91204100	H	-1.64582500	-1.45340300	-1.73645500
H	-2.57506600	0.27696300	2.61423200	H	-3.11663100	-2.16020600	-1.03849500
H	-2.11897200	-1.33224300	3.22398300	H	-3.10022000	-1.60710900	-2.72520900
H	-2.86881600	-3.38746400	1.99220300	H	-3.37004900	0.82738000	-3.26649700
H	-3.17728200	-3.33713000	0.25989400	H	-2.98066400	2.06877100	-2.07974900
H	-1.57577500	-2.91279000	0.90415200	H	-1.73268800	0.93400600	-2.63014900
H	-1.63659900	-1.71279000	-0.82618100	H	0.64236200	2.72709900	-2.38199000
H	1.72866400	-3.42389100	-1.35769600	H	-1.04330600	1.41732600	-0.63508000
14				15			
Charge=1 Multiplicity = 1				Charge=1 Multiplicity = 1			
Cu	-0.38470100	0.00590200	0.05451200	O	-0.55617800	-1.39667200	2.41369400
N	1.07597900	1.31794100	-0.12246600	O	-0.84546900	-2.04661000	1.31080400
N	1.08769400	-1.31290300	0.10844600	Cu	-0.24688100	-0.45285500	0.42515000
C	3.46323600	1.51860900	0.06212200	N	1.53671700	-1.17046900	-0.18937400
C	2.30474500	0.74706200	-0.04047500	C	2.48161900	-0.21638000	-0.35735600
C	2.09613700	3.49241600	-0.01480200	C	1.84726200	-2.45767500	-0.38969600
H	4.24925600	3.52267000	0.15638600	C	3.77643900	-0.54804200	-0.75932700
H	-0.01736600	3.06558700	-0.18218400	C	2.02718000	1.16817100	-0.06772300
H	1.96743700	4.56932900	-0.01148800	C	3.11821100	-2.86240200	-0.79127900

H	4.43562500	1.04817500	0.15000800	H	1.04980400	-3.17183700	-0.21165100
H	4.23751800	-3.51121000	-0.39475100	H	4.53232800	0.21672400	-0.89271500
C	3.35301800	-2.89874500	-0.24995400	C	4.09519300	-1.88747900	-0.98125200
C	2.10220300	-3.48523400	-0.06960300	N	0.73781700	1.27898500	0.33771900
C	3.45599000	-1.50860400	-0.24716400	C	2.84315700	2.29668600	-0.17074200
C	0.99937700	-2.65276900	0.10229400	H	3.32961300	-3.91480500	-0.94516200
H	1.97621200	-4.56245200	-0.06149600	H	5.09799100	-2.16256900	-1.29286700
C	2.30590500	-0.73970600	-0.06224500	C	0.24068600	2.48374500	0.65432000
H	4.41870800	-1.03621800	-0.40435800	C	2.32446900	3.54731100	0.15951900
C	3.35796100	2.90846100	0.07422100	H	3.87162400	2.20795600	-0.49954400
H	0.00539800	-3.06269000	0.25038200	C	1.00066000	3.64724900	0.58414500
C	0.98560600	2.65785300	-0.10801300	H	-0.79742200	2.50215300	0.97049900
N	-2.25289000	-0.01423300	0.19728000	H	2.95045600	4.43128500	0.08768700
C	-2.96381300	-0.17459500	1.37547600	H	0.56199400	4.60072100	0.85672800
C	-3.16553000	0.10417800	-0.76485100	N	-2.04003600	0.02214500	-0.28433200
C	-4.30314000	-0.14993300	1.10269800	C	-2.39755500	0.95517500	-1.23931900
H	-2.47045600	-0.29619900	2.32774600	C	-3.16821800	-0.57930100	0.08403100
N	-4.41864900	0.02583700	-0.25990700	C	-3.74951600	0.90330100	-1.43646800
H	-2.96295100	0.24654100	-1.81595100	H	-1.66603400	1.58550000	-1.72211700
H	-5.16828400	-0.24017900	1.74161200	N	-4.22521200	-0.07681900	-0.58736300
C	-5.66405400	0.10985500	-1.01866500	H	-3.24140000	-1.37177300	0.81392600
H	-6.23563300	-0.81507100	-0.90688900	H	-4.40333000	1.45843200	-2.09176000
H	-6.26256700	0.95369400	-0.66604000	C	-5.61899200	-0.49492800	-0.44323600
H	-5.42735400	0.25730000	-2.07352700	H	-6.23082400	0.34871100	-0.11438700
				H	-5.99650500	-0.87193200	-1.39694300
				H	-5.67414200	-1.28897300	0.30273300
15				16			
Charge=1 Multiplicity =3				Charge=1 Multiplicity = 3			
O	-0.52716800	-1.30873300	2.48115500	Cu	-2.23682100	0.38550100	-0.16246700
O	-0.85063700	-1.98973500	1.42232900	N	-2.88913200	-1.10288400	1.00400600
Cu	-0.25563300	-0.43411200	0.44838700	N	-4.18084800	0.38491900	-0.72841500
N	1.50647500	-1.18603900	-0.20006700	C	-4.81837700	-2.32371700	1.72344000
C	2.46614600	-0.24620500	-0.36868400	C	-4.21784300	-1.35197000	0.92044600
C	1.79946500	-2.47667900	-0.40742100	C	-2.66233200	-2.79202700	2.68422300
C	3.75543300	-0.59701700	-0.77355000	H	-4.48565700	-3.80069900	3.25460000
C	2.03777300	1.14747300	-0.07933400	H	-1.07260500	-1.57092700	1.84371300
C	3.06280500	-2.90019400	-0.81272000	H	-2.01803500	-3.33593900	3.36638600
H	0.99275300	-3.18156100	-0.23364000	H	-5.88248800	-2.51781800	1.66056900
H	4.52301000	0.15639000	-0.90431700	H	-7.94389800	0.07418900	-1.54882000
C	4.05451400	-1.93980500	-1.00028900	C	-6.88635200	0.16458300	-1.32126900
N	0.75896200	1.28246000	0.35081900	C	-6.09081700	1.08987700	-1.99482100
C	2.86923600	2.26206400	-0.21080800	C	-6.30865600	-0.65038200	-0.34861400
H	3.25719300	-3.95516200	-0.97156100	C	-4.74171600	1.16903900	-1.66069300
H	5.05281600	-2.22875000	-1.31378200	H	-6.50091900	1.73868700	-2.76091400

C	0.28743200	2.49894000	0.66193500	C	-4.94620000	-0.52191100	-0.07227900
C	2.37737400	3.52416600	0.11622500	H	-6.91743000	-1.37441300	0.17975300
H	3.88867700	2.15447300	-0.56129400	C	-4.03149600	-3.04718600	2.61863600
C	1.06365500	3.64966700	0.56476400	H	-4.07989500	1.87958100	-2.14522300
H	-0.74425700	2.53788000	0.99707500	C	-2.13031400	-1.81027500	1.85265800
H	3.01565800	4.39720100	0.02219900	O	-0.58015900	-0.38231700	-0.49548900
H	0.64512000	4.61290300	0.83477000	O	0.58038400	0.38508400	-0.49220600
N	-2.04444900	0.01647500	-0.28370400	Cu	2.23643600	-0.38486600	-0.16153900
C	-2.38560800	0.94092200	-1.25277100	N	2.89115700	1.10283300	1.00480500
C	-3.18092000	-0.57219000	0.07859000	C	4.21991000	1.35113000	0.91958600
C	-3.73577500	0.89685800	-1.46422100	C	2.13381500	1.81082300	1.85428000
H	-1.64440800	1.56146200	-1.73350200	C	4.82200000	2.32267400	1.72166600
N	-4.22779700	-0.07015400	-0.60972600	C	4.94659700	0.52046900	-0.07385500
H	-3.27040400	-1.35408300	0.81818400	C	2.66741900	2.79241300	2.68501600
H	-4.37856600	1.44967000	-2.13224900	H	1.07595400	1.57210600	1.84665700
C	-5.62605500	-0.47580900	-0.47537200	H	5.88613900	2.51618100	1.65743600
H	-6.23431800	0.37515000	-0.15889900	C	4.03664700	3.04676300	2.61769800
H	-5.99785100	-0.85734700	-1.42953800	N	4.17987800	-0.38577600	-0.72920400
H	-5.69481000	-1.26356100	0.27617200	C	6.30889000	0.64781700	-0.35153400
				H	2.02427400	3.33682100	3.36787100
				H	4.49202700	3.80013400	3.25296000
				C	4.73922300	-1.17042700	-1.66195500
				C	6.88498600	-0.16767400	-1.32469200
				H	6.91876700	1.37136600	0.17621600
				C	6.08805600	-1.09238400	-1.99739700
				H	4.07637100	-1.88046500	-2.14581400
				H	7.94238500	-0.07814700	-1.55327100
				H	6.49689500	-1.74158700	-2.76383000
				N	1.89699600	-2.33287400	-0.20129100
				C	2.74484600	-3.33734600	0.23316500
				C	0.87428900	-2.94293800	-0.79511200
				C	2.21475800	-4.55117500	-0.10349900
				H	3.66356600	-3.12217400	0.75789800
				N	1.02716700	-4.28411500	-0.75818800
				H	0.02722900	-2.43091000	-1.22667000
				H	2.56335700	-5.55943200	0.06190700
				C	0.11624400	-5.27687700	-1.32630100
				H	0.62754100	-5.85683500	-2.09865600
				H	-0.24030500	-5.95064500	-0.54315800
				H	-0.73489900	-4.76089100	-1.77300700
				N	-1.89881400	2.33380600	-0.20234600
				C	-2.74756100	3.33789400	0.23123900
				C	-0.87565200	2.94433900	-0.79489600
				C	-2.21755900	4.55196800	-0.10466000

H	-3.66676700	3.12230400	0.75494700
N	-1.02909100	4.28544600	-0.75797700
H	-0.02782600	2.43273900	-1.22545600
H	-2.56674300	5.56007000	0.06045400
C	-0.11803000	5.27862300	-1.32514400
H	-0.62818400	5.85712100	-2.09935600
H	0.23588600	5.95367300	-0.54192100
H	0.73477200	4.76312400	-1.76924000

17	Charge=2 Multiplicity =1			17	Charge=2 Multiplicity = 3		
Cu	-2.22463700	-0.85574200	0.23776700	Cu	-2.20414100	-0.88961800	0.23694900
N	-2.33176300	-1.93629000	-1.43619400	N	-2.24673900	-1.95175800	-1.44391900
N	-4.23972000	-0.94467000	0.04269000	N	-4.21044200	-1.02511500	0.00418800
C	-3.78383800	-2.95452700	-3.04030600	C	-3.63863000	-2.99174400	-3.08690200
C	-3.58114200	-2.20782400	-1.87881000	C	-3.47979300	-2.25262100	-1.91387600
C	-1.39349000	-3.12452200	-3.28171400	C	-1.24044500	-3.09014100	-3.28548500
H	-2.81381300	-4.00347700	-4.65095900	H	-2.60938800	-3.99407800	-4.69047000
H	-0.30372900	-2.09631700	-1.69304400	H	-0.20990600	-2.04894200	-1.66861000
H	-0.51033100	-3.46862000	-3.80881400	H	-0.33781100	-3.40093000	-3.80005800
H	-4.78370900	-3.17303700	-3.39625400	H	-4.62506300	-3.23446400	-3.46398100
H	-8.02141400	-1.30076300	-0.66158000	H	-7.96637300	-1.48462800	-0.77342200
C	-6.95958100	-1.19771900	-0.46083700	C	-6.91185900	-1.35264300	-0.55211100
C	-6.51182300	-0.47079800	0.64056100	C	-6.50582800	-0.62211600	0.56295500
C	-6.02692400	-1.79370300	-1.30939300	C	-5.94682400	-1.91465800	-1.38767000
C	-5.13984500	-0.37476000	0.85748700	C	-5.14138900	-0.48817700	0.80648600
H	-7.20483800	0.01080400	1.32157000	H	-7.22505000	-0.16613000	1.23435400
C	-4.66644000	-1.64745000	-1.03598500	C	-4.59661900	-1.73129700	-1.08751700
H	-6.36248900	-2.36041100	-2.16982000	H	-6.25000400	-2.48401000	-2.25834600
C	-2.67443600	-3.41914900	-3.74665400	C	-2.50354000	-3.41646100	-3.77736200
H	-4.73666000	0.16861400	1.70539600	H	-4.76950600	0.05973700	1.66565400
C	-1.26339400	-2.37022700	-2.11799700	C	-1.15415100	-2.34666000	-2.11097500
O	-0.52532600	-0.14880600	-0.12852700	O	-0.52167300	-0.11622100	-0.07460700
O	0.47391400	-1.05636600	0.35000800	O	0.49261200	-0.97678300	0.44573000
Cu	2.19032100	-0.88701900	-0.29589700	Cu	2.18861400	-0.87709700	-0.26935800
N	2.75167900	-2.58469000	0.64799400	N	2.75681400	-2.56509900	0.68854300
C	4.06359700	-2.64768100	0.97434500	C	4.07176600	-2.62075300	1.00527600
C	1.92991400	-3.58410300	0.99613200	C	1.94001600	-3.55914800	1.06343400
C	4.58420400	-3.75097100	1.65388700	C	4.59956600	-3.71090300	1.70038300
C	4.86251400	-1.46903500	0.55826400	C	4.86658900	-1.44777700	0.56510200
C	2.37988000	-4.71522400	1.67142100	C	2.39701500	-4.67701000	1.75576900
H	0.88971700	-3.44254900	0.72430600	H	0.89676500	-3.42578300	0.79993300

H	5.63447300	-3.79894100	1.91584500	H	5.65191600	-3.75237100	1.95495300
C	3.73196800	-4.79807800	2.00108500	C	3.75209100	-4.75251900	2.07450400
N	4.15352600	-0.48781000	-0.05265000	N	4.15141200	-0.47220300	-0.04756000
C	6.23586900	-1.33979800	0.77336200	C	6.24250700	-1.31701700	0.76286400
H	1.68561500	-5.50711100	1.93036700	H	1.70581800	-5.46432100	2.03602200
H	4.12187200	-5.66428200	2.52658100	H	4.14778600	-5.60826500	2.61263300
C	4.78297400	0.62545800	-0.45696500	C	4.77602200	0.63772900	-0.46811300
C	6.88457600	-0.17827600	0.35718400	C	6.88654100	-0.15942300	0.32899200
H	6.79859900	-2.13000300	1.25583200	H	6.81085400	-2.10295500	1.24569600
C	6.14704500	0.82618100	-0.26675900	C	6.14204300	0.84008100	-0.29478200
H	4.16364300	1.37096800	-0.94309600	H	4.15100500	1.37948700	-0.95306100
H	7.95173100	-0.06300400	0.51925400	H	7.95550400	-0.04303700	0.47778400
H	6.61299300	1.74585300	-0.60297300	H	6.60416600	1.75712300	-0.64325300
N	1.96328900	-0.01319600	-2.05089000	N	1.94033100	-0.04463900	-2.04277500
C	2.62170900	-0.38976400	-3.20932400	C	2.60324000	-0.41586100	-3.20039300
C	1.23314000	1.05492600	-2.36499700	C	1.20281300	1.01835900	-2.35873600
C	2.27252800	0.46041500	-4.22038200	C	2.24923800	0.43169600	-4.21220600
H	3.29370500	-1.23485700	-3.23682700	H	3.28232600	-1.25530700	-3.22641400
N	1.39443300	1.37287300	-3.66849100	N	1.36337500	1.33759800	-3.66186400
H	0.61733400	1.62676100	-1.68237600	H	0.57937900	1.58269200	-1.67767800
H	2.56028600	0.49940900	-5.26011700	H	2.53877700	0.47307100	-5.25137200
C	0.77248000	2.49660000	-4.36845800	C	0.73387800	2.45739000	-4.36162100
H	1.54198800	3.17782800	-4.74037000	H	1.49872100	3.14567500	-4.73011500
H	0.17609000	2.13033100	-5.20789600	H	0.14290300	2.08769700	-5.20336300
H	0.12513900	3.02994500	-3.67194500	H	0.08040900	2.98414100	-3.66566600
N	-2.14569000	-0.78402200	2.20832800	N	-2.16402600	-0.81182800	2.21150400
C	-2.76062200	-1.66441200	3.08248600	C	-2.76303400	-1.70498900	3.08357200
C	-1.43250100	0.05264500	2.95930000	C	-1.49662600	0.05816700	2.96674500
C	-2.40603800	-1.34479300	4.36282500	C	-2.44465200	-1.35980000	4.36687700
H	-3.40424200	-2.45964900	2.73654300	H	-3.37107300	-2.52640400	2.73428800
N	-1.56606700	-0.25194000	4.26683300	N	-1.64375400	-0.23771000	4.27474900
H	-0.84113900	0.88286900	2.59357200	H	-0.92663300	0.90467700	2.60498700
H	-2.66711100	-1.78559500	5.31298800	H	-2.70752000	-1.80009000	5.31678900
C	-0.94125200	0.45752400	5.38287100	C	-1.06558600	0.50539700	5.39415000
H	-1.70915400	0.85137300	6.05323000	H	-1.85954700	0.88141900	6.04407600
H	-0.28611900	-0.21917700	5.93717000	H	-0.39984000	-0.14263200	5.96960600
H	-0.35167200	1.28535800	4.98672500	H	-0.49549100	1.34739400	4.99936300
H	1.70360500	6.19411900	0.06038700	H	1.66946000	6.22129800	0.00440900
C	0.84628100	5.54103500	-0.13678600	C	0.80710000	5.57068800	-0.17854100
C	-0.46749600	6.25917000	0.23522500	C	-0.50098200	6.30564800	0.18039900
C	1.06374800	4.21465400	0.61430400	C	1.01609000	4.25806200	0.59924200
H	0.87181900	5.32897800	-1.21307500	H	0.82934900	5.33695600	-1.25046100
H	-0.80607300	6.84943800	-0.62313700	H	-0.83697700	6.87966900	-0.68992900
C	-1.57085900	5.27713900	0.68093900	C	-1.61064800	5.34137900	0.64832700

H	-0.28816900	6.97925300	1.04042600	H	-0.31548500	7.04163400	0.96966400
N	-0.03862700	3.27995800	0.20899700	N	-0.09520000	3.32456200	0.21739900
C	-1.43741600	3.86784800	0.06065500	C	-1.48898500	3.91853200	0.05710400
H	-2.55782600	5.67822300	0.42191000	H	-2.59513800	5.74468400	0.38335300
H	-1.57007000	5.17571500	1.77101200	H	-1.60801100	5.26187500	1.74022400
O	-0.00758400	2.18593500	1.15589100	O	-0.07270000	2.25024400	1.18609400
C	-2.49140400	2.95263700	0.69930800	C	-2.54955900	3.02477100	0.71533000
H	-2.44798500	1.93995000	0.28089800	H	-2.51733100	2.00443600	0.31492200
H	-2.36857600	2.88231000	1.78237700	H	-2.42384500	2.97279000	1.79909500
H	-3.48604300	3.36122900	0.48971600	H	-3.54091100	3.43928500	0.50174500
C	-1.72758800	3.93190600	-1.45564900	C	-1.77885800	3.95267500	-1.46029800
H	-2.72889900	4.33732900	-1.64242100	H	-2.77631200	4.36333100	-1.65616800
H	-1.01108100	4.56742400	-1.98400300	H	-1.05584300	4.56905800	-2.00222800
H	-1.68228700	2.92666000	-1.89265200	H	-1.74253900	2.93754300	-1.87488400
C	1.17114800	4.45268800	2.13897600	C	1.13029700	4.52718700	2.11813000
H	1.35564000	3.51167200	2.66181800	H	1.30181300	3.59508100	2.66085400
H	2.01186700	5.12549800	2.34143600	H	1.98066700	5.19235800	2.30505600
H	0.27683200	4.90883900	2.56763400	H	0.24310400	5.00518600	2.53778300
C	2.38567600	3.58096200	0.14372700	C	2.33055500	3.60263100	0.13692400
H	2.52963400	2.60559900	0.62025800	H	2.46811500	2.63602700	0.63317600
H	2.38580800	3.44791700	-0.94451100	H	2.32377200	3.44646400	-0.94829100
H	3.23496800	4.21989500	0.41056400	H	3.18677300	4.23944300	0.38619000
H	-0.11916800	1.37627800	0.59854600	H	-0.15795600	1.43221900	0.63960500
TS17-18				TS17-18			
Charge=2 Multiplicity =1				Charge=2 Multiplicity = 3			
Cu	-2.10345500	-0.80590100	0.45829300	Cu	-2.20793800	-0.79571800	0.34498600
N	-1.97785700	-2.51416000	-0.65863300	N	-2.30903900	-2.06890200	-1.18605100
N	-4.02391200	-0.93952700	-0.12160100	N	-4.20083500	-0.65898500	-0.01692300
C	-3.22541500	-3.94516500	-2.12933900	C	-3.75865400	-2.98896000	-2.86047800
C	-3.15448600	-2.88195800	-1.22209500	C	-3.55045300	-2.22533200	-1.70779400
C	-0.85593700	-4.25412600	-1.87205500	C	-1.39555500	-3.43130300	-2.93281700
H	-2.10580600	-5.47761700	-3.14530700	H	-2.81741600	-4.20622500	-4.36605900
H	0.04836500	-2.81351000	-0.52334000	H	-0.29861100	-2.45978700	-1.32495200
H	0.06980500	-4.77349700	-2.09622000	H	-0.52438500	-3.89728600	-3.38099200
H	-4.16775500	-4.21926600	-2.58927200	H	-4.75133900	-3.09597800	-3.28209600
H	-7.71133900	-1.83075500	-0.90860200	H	-7.99054400	-1.20669000	-0.60372700
C	-6.67912000	-1.57587800	-0.69006000	C	-6.92935800	-1.04861300	-0.43899500
C	-6.36492600	-0.41316200	0.01568700	C	-6.48410900	-0.15101700	0.53198200
C	-5.64717600	-2.41318100	-1.10461300	C	-5.99076500	-1.75002200	-1.19203100
C	-5.02813100	-0.14201200	0.28373900	C	-5.11364500	0.00329700	0.71272800
H	-7.13672100	0.26924100	0.35504800	H	-7.18051400	0.41660200	1.13972700
C	-4.32336300	-2.06946100	-0.81342500	C	-4.62919000	-1.53336600	-0.96358600
H	-5.87529600	-3.33078000	-1.63426900	H	-6.31992500	-2.46811000	-1.93410300

C	-2.06585800	-4.64480600	-2.45004000	C	-2.67065200	-3.60408000	-3.47471900
H	-4.73404300	0.74164000	0.84119000	H	-4.71778900	0.68081100	1.46268400
C	-0.85999600	-3.17899000	-0.99048900	C	-1.26004300	-2.64726600	-1.79209000
O	-0.46189500	0.10146400	-0.17081500	O	-0.49581500	0.06235800	-0.10086500
O	0.62808900	-0.50933100	0.56064700	O	0.54510000	-0.80344800	0.39348000
Cu	2.30127100	-0.62688700	-0.21503000	Cu	2.24814900	-0.76001300	-0.32526800
N	2.96312200	-1.75604100	1.32450900	N	2.81955600	-2.27042600	0.89663300
C	4.29775500	-1.69711100	1.54294200	C	4.13767800	-2.28457400	1.20237300
C	2.19370700	-2.52822600	2.10429500	C	2.00462600	-3.19550300	1.42174900
C	4.89587200	-2.45144900	2.55408700	C	4.67339100	-3.26677700	2.03806000
C	5.03378900	-0.77717900	0.64087700	C	4.92779500	-1.18535900	0.59471000
C	2.72225500	-3.30726200	3.13046100	C	2.46948100	-4.20556700	2.25992800
H	1.13125200	-2.49259400	1.88882000	H	0.95687600	-3.09450800	1.16034500
H	5.96509100	-2.40768900	2.72385200	H	5.72916900	-3.27706000	2.28130100
C	4.09784200	-3.26994700	3.35255700	C	3.82870000	-4.24168900	2.56687800
N	4.26584000	-0.14857700	-0.28331800	N	4.21176900	-0.31386600	-0.15875000
C	6.40625500	-0.53367300	0.72354500	C	6.30172000	-1.01724000	0.78039500
H	2.06818200	-3.92539600	3.73567200	H	1.77997700	-4.94141100	2.65904500
H	4.54833200	-3.86629300	4.13990000	H	4.22996400	-5.01474000	3.21485800
C	4.83426300	0.72616600	-1.12734700	C	4.83520100	0.72794300	-0.73070100
C	6.99185800	0.37607700	-0.15527600	C	6.94358700	0.06797600	0.18662000
H	7.01595200	-1.03992600	1.46229900	H	6.87010600	-1.71937500	1.37847300
C	6.19340900	1.02357400	-1.09677200	C	6.19864700	0.96209100	-0.58065700
H	4.16958300	1.19293800	-1.84665700	H	4.21113500	1.38670400	-1.32511700
H	8.05744900	0.57607900	-0.10133600	H	8.01090300	0.21085500	0.32381300
H	6.60949200	1.74107800	-1.79542300	H	6.65886500	1.82098700	-1.05663200
N	1.95264600	-0.62829400	-2.15687900	N	1.98635600	-0.29473700	-2.22461500
C	2.78681500	-1.13867700	-3.13771300	C	2.87258800	-0.51229900	-3.26560700
C	0.87357400	-0.17102300	-2.78699400	C	0.90917900	0.26827300	-2.76494500
C	2.19200600	-0.98210600	-4.35787800	C	2.31157300	-0.07272900	-4.43180600
H	3.74187300	-1.58364500	-2.90263100	H	3.83786400	-0.96945500	-3.10914900
N	0.97909800	-0.36434100	-4.11840100	N	1.06543600	0.42199700	-4.09714400
H	0.02589600	0.27123200	-2.28402500	H	0.02513100	0.53918200	-2.20558600
H	2.51230500	-1.24944200	-5.35356200	H	2.67593800	-0.06745400	-5.44800700
C	-0.00870500	0.01334400	-5.12844600	C	0.09445200	1.00414000	-5.02246100
H	0.43631100	0.70635600	-5.84668000	H	0.54396500	1.84634000	-5.55409200
H	-0.36624400	-0.87537000	-5.65451300	H	-0.23497700	0.25324000	-5.74516000
H	-0.84954800	0.50146800	-4.63375500	H	-0.76611200	1.35946400	-4.45387400
N	-2.23336000	-0.36776500	2.36599900	N	-2.11962000	-0.76256600	2.32460300
C	-3.26187500	-0.66481900	3.24205700	C	-2.87349400	-1.50785000	3.21310700
C	-1.34125700	0.32263200	3.06950800	C	-1.31667700	-0.00795100	3.06740000
C	-2.97408400	-0.14554400	4.47298700	C	-2.51049900	-1.19221200	4.49310900
H	-4.12503000	-1.23540700	2.93459300	H	-3.61555800	-2.21638000	2.87621800
N	-1.74837900	0.48027400	4.34822800	N	-1.52003700	-0.23515600	4.38449500

H	-0.41611200	0.71690400	2.68014900	H	-0.60575800	0.71255000	2.68684700
H	-3.51308300	-0.16605900	5.40801600	H	-2.85669500	-1.55184400	5.45031400
C	-1.04034500	1.20366600	5.40099200	C	-0.83419700	0.42468600	5.49277000
H	-1.63655400	2.05467500	5.74032700	H	-1.55172300	0.97613200	6.10592300
H	-0.84237800	0.53975100	6.24643900	H	-0.32220800	-0.31580900	6.11268000
H	-0.09259100	1.56909400	5.00258600	H	-0.09917700	1.12218200	5.08817100
H	1.81942600	5.52481000	-0.76461500	H	1.60516000	6.09488700	-0.48949200
C	0.86753000	5.01825000	-0.95888100	C	0.75419500	5.40760400	-0.54646800
C	-0.26792500	6.05207100	-1.10934200	C	-0.55509100	6.15010700	-0.20547600
C	0.64431700	3.97689200	0.15388800	C	1.05691700	4.19700100	0.35647500
H	1.00096800	4.47387400	-1.90177000	H	0.72330500	5.05213000	-1.58359100
H	-0.31868600	6.36538300	-2.15729800	H	-0.95966400	6.58719200	-1.12435900
C	-1.63620200	5.51618200	-0.64163800	C	-1.60590100	5.24176500	0.46410200
H	-0.03502900	6.95717000	-0.53917800	H	-0.35084800	6.99436000	0.46080400
N	-0.64895900	3.29574700	-0.11034600	N	-0.10222600	3.27073500	0.27909000
C	-1.81430600	3.98362200	-0.75008800	C	-1.51048300	3.74717300	0.07874500
H	-2.44141700	5.98939800	-1.21442100	H	-2.61583100	5.59009900	0.21954800
H	-1.80861300	5.79460100	0.40360700	H	-1.51948800	5.30894100	1.55395700
O	-0.94415700	2.28584400	0.74526300	O	0.08444100	2.13029900	0.98529100
C	-3.11938800	3.58847500	-0.04243700	C	-2.47436200	2.94489300	0.96328500
H	-3.34109900	2.52613500	-0.16923400	H	-2.50353800	1.88802200	0.68081900
H	-3.07228500	3.80440700	1.02822600	H	-2.19805200	3.01068600	2.01900400
H	-3.94145800	4.16578700	-0.47805300	H	-3.48226600	3.35517800	0.84175700
C	-1.88380100	3.53166500	-2.22806600	C	-1.89474700	3.53217400	-1.40415700
H	-2.76110300	3.97095500	-2.71586300	H	-2.93532400	3.83238100	-1.57110200
H	-0.99672000	3.83424100	-2.79173000	H	-1.26427800	4.11468800	-2.08136100
H	-1.97410500	2.44027900	-2.28447700	H	-1.79955500	2.47271100	-1.67052400
C	0.64903700	4.61539300	1.56274100	C	1.33616100	4.61835900	1.81783400
H	0.38875500	3.86336600	2.31278200	H	1.45757300	3.73137000	2.44573600
H	1.64695600	5.00496400	1.79139500	H	2.26080400	5.20362700	1.86425100
H	-0.05935800	5.44269300	1.64678300	H	0.53330700	5.23060600	2.23568700
C	1.76353100	2.92076500	0.08280600	C	2.29063600	3.45389200	-0.19024700
H	1.62125300	2.14569800	0.84035200	H	2.55552500	2.61348100	0.45678700
H	1.77591000	2.44685800	-0.90584400	H	2.09424100	3.07565400	-1.20029700
H	2.73374400	3.40004500	0.25099000	H	3.14325100	4.13964300	-0.23634500
H	-0.62428800	1.28383100	0.30172600	H	-0.20885900	1.17730900	0.40014000
18				18			
Charge=2 Multiplicity =1				Charge=2 Multiplicity = 3			
Cu	-2.22463700	-0.85574200	0.23776700	Cu	-2.42515400	-0.34928200	0.66277200
N	-2.33176300	-1.93629000	-1.43619400	N	-2.78782500	-2.23707500	0.12386300
N	-4.23972000	-0.94467000	0.04269000	N	-4.25086800	-0.04154800	-0.11278500
C	-3.78383800	-2.95452700	-3.04030600	C	-4.40944400	-3.62668400	-0.98605700
C	-3.58114200	-2.20782400	-1.87881000	C	-4.02092000	-2.40739200	-0.41916300

C	-1.39349000	-3.12452200	-3.28171400	C	-2.24387600	-4.51012700	-0.44347200
H	-2.81381300	-4.00347700	-4.65095900	H	-3.80499900	-5.64765000	-1.41994400
H	-0.30372900	-2.09631700	-1.69304400	H	-0.94926700	-3.06611600	0.52482300
H	-0.51033100	-3.46862000	-3.80881400	H	-1.51746600	-5.31603300	-0.42319200
H	-4.78370900	-3.17303700	-3.39625400	H	-5.39138200	-3.73818200	-1.43175500
H	-8.02141400	-1.30076300	-0.66158000	H	-8.10378400	-0.12356400	-0.61304200
C	-6.95958100	-1.19771900	-0.46083700	C	-7.02699400	-0.09679900	-0.47916000
C	-6.51182300	-0.47079800	0.64056100	C	-6.36683000	1.10591300	-0.22257400
C	-6.02692400	-1.79370300	-1.30939300	C	-6.27936600	-1.26837400	-0.54950500
C	-5.13984500	-0.37476000	0.85748700	C	-4.98872000	1.08227800	-0.04295600
H	-7.20483800	0.01080400	1.32157000	H	-6.90664200	2.04506200	-0.16207600
C	-4.66644000	-1.64745000	-1.03598500	C	-4.89352900	-1.21341900	-0.36834300
H	-6.36248900	-2.36041100	-2.16982000	H	-6.77453500	-2.21792900	-0.71842700
C	-2.67443600	-3.41914900	-3.74665400	C	-3.51573000	-4.69298300	-0.99147200
H	-4.73666000	0.16861400	1.70539600	H	-4.43889400	1.99526900	0.16335600
C	-1.26339400	-2.37022700	-2.11799700	C	-1.92460600	-3.26859200	0.09429100
O	-0.52532600	-0.14880600	-0.12852700	O	-0.52556100	-0.13817900	-0.23167000
O	0.47391400	-1.05636600	0.35000800	O	0.44787000	-0.80438100	0.62325200
Cu	2.19032100	-0.88701900	-0.29589700	Cu	2.09804500	-1.21099800	-0.11347400
N	2.75167900	-2.58469000	0.64799400	N	2.76958700	-1.82574700	1.68403200
C	4.06359700	-2.64768100	0.97434500	C	4.11137500	-1.74934500	1.84413800
C	1.92991400	-3.58410300	0.99613200	C	2.00291700	-2.29470700	2.67791600
C	4.58420400	-3.75097100	1.65388700	C	4.72043900	-2.17980000	3.02389300
C	4.86251400	-1.46903500	0.55826400	C	4.84092700	-1.17296200	0.68745600
C	2.37988000	-4.71522400	1.67142100	C	2.54285000	-2.74216500	3.88136700
H	0.88971700	-3.44254900	0.72430600	H	0.93485900	-2.28960200	2.48776600
H	5.63447300	-3.79894100	1.91584500	H	5.79527900	-2.12450400	3.14923700
C	3.73196800	-4.79807800	2.00108500	C	3.92513400	-2.68756600	4.05103400
N	4.15352600	-0.48781000	-0.05265000	N	4.06089500	-0.83398100	-0.36909700
C	6.23586900	-1.33979800	0.77336200	C	6.22026800	-0.95685800	0.66134000
H	1.68561500	-5.50711100	1.93036700	H	1.89170700	-3.12254000	4.66071200
H	4.12187200	-5.66428200	2.52658100	H	4.38358500	-3.03121200	4.97309200
C	4.78297400	0.62545800	-0.45696500	C	4.62248000	-0.27583200	-1.45278100
C	6.88457600	-0.17827600	0.35718400	C	6.79925800	-0.37708600	-0.46616500
H	6.79859900	-2.13000300	1.25583200	H	6.84031100	-1.23197000	1.50616700
C	6.14704500	0.82618100	-0.26675900	C	5.98793100	-0.02382300	-1.54364000
H	4.16364300	1.37096800	-0.94309600	H	3.94686800	-0.03561600	-2.26737600
H	7.95173100	-0.06300400	0.51925400	H	7.87030400	-0.20339900	-0.49933300
H	6.61299300	1.74585300	-0.60297300	H	6.39931800	0.43187000	-2.43758700
N	1.96328900	-0.01319600	-2.05089000	N	1.65891300	-1.83716300	-1.93204100
C	2.62170900	-0.38976400	-3.20932400	C	2.47395700	-2.60179900	-2.75000800
C	1.23314000	1.05492600	-2.36499700	C	0.48917000	-1.74050000	-2.56014600
C	2.27252800	0.46041500	-4.22038200	C	1.77869700	-2.95548300	-3.87177100
H	3.29370500	-1.23485700	-3.23682700	H	3.48745400	-2.85222900	-2.47628400

N	1.39443300	1.37287300	-3.66849100	N	0.52130100	-2.39968700	-3.73665200
H	0.61733400	1.62676100	-1.68237600	H	-0.36998000	-1.21595600	-2.16952600
H	2.56028600	0.49940900	-5.26011700	H	2.05652200	-3.54173500	-4.73459800
C	0.77248000	2.49660000	-4.36845800	C	-0.57487400	-2.50740000	-4.69908700
H	1.54198800	3.17782800	-4.74037000	H	-0.28211700	-2.06040200	-5.65236200
H	0.17609000	2.13033100	-5.20789600	H	-0.83372500	-3.55767800	-4.85353000
H	0.12513900	3.02994500	-3.67194500	H	-1.44348800	-1.97771500	-4.30553200
N	-2.14569000	-0.78402200	2.20832800	N	-2.20891800	0.60815000	2.34675500
C	-2.76062200	-1.66441200	3.08248600	C	-3.11069000	0.61708500	3.39562500
C	-1.43250100	0.05264500	2.95930000	C	-1.22238700	1.42047300	2.71038800
C	-2.40603800	-1.34479300	4.36282500	C	-2.65252100	1.43943300	4.38777700
H	-3.40424200	-2.45964900	2.73654300	H	-4.01836800	0.03312500	3.36783200
N	-1.56606700	-0.25194000	4.26683300	N	-1.44947900	1.94609200	3.93890600
H	-0.84113900	0.88286900	2.59357200	H	-0.35075200	1.65653200	2.11634200
H	-2.66711100	-1.78559500	5.31298800	H	-3.06145700	1.70448800	5.35104800
C	-0.94125200	0.45752400	5.38287100	C	-0.58766200	2.87937200	4.65619600
H	-1.70915400	0.85137300	6.05323000	H	-1.12567800	3.80786900	4.86537700
H	-0.28611900	-0.21917700	5.93717000	H	-0.25146300	2.43844100	5.59862000
H	-0.35167200	1.28535800	4.98672500	H	0.28302300	3.10356200	4.03734000
H	1.70360500	6.19411900	0.06038700	H	2.64281600	5.84553900	-1.76071700
C	0.84628100	5.54103500	-0.13678600	C	1.87217900	5.07928000	-1.89779700
C	-0.46749600	6.25917000	0.23522500	C	0.60550200	5.70182900	-2.52303700
C	1.06374800	4.21465400	0.61430400	C	1.65469000	4.37570700	-0.54217700
H	0.87181900	5.32897800	-1.21307500	H	2.30028200	4.34017200	-2.58584900
H	-0.80607300	6.84943800	-0.62313700	H	0.69122500	5.64537500	-3.61303200
C	-1.57085900	5.27713900	0.68093900	C	-0.70016000	5.02859400	-2.05401700
H	-0.28816900	6.97925300	1.04042600	H	0.54725400	6.76841300	-2.28423000
N	-0.03862700	3.27995800	0.20899700	N	0.55734800	3.36560700	-0.72251600
C	-1.43741600	3.86784800	0.06065500	C	-0.57985600	3.53572600	-1.68511200
H	-2.55782600	5.67822300	0.42191000	H	-1.46835800	5.11654300	-2.82995800
H	-1.57007000	5.17571500	1.77101200	H	-1.09900200	5.55732600	-1.18151300
O	-0.00758400	2.18593500	1.15589100	O	0.62973700	2.27302100	-0.03616200
C	-2.49140400	2.95263700	0.69930800	C	-1.88397500	3.09201100	-0.99800300
H	-2.44798500	1.93995000	0.28089800	H	-1.90870900	2.02023700	-0.78221900
H	-2.36857600	2.88231000	1.78237700	H	-2.03254800	3.63467900	-0.05868500
H	-3.48604300	3.36122900	0.48971600	H	-2.72567700	3.31874400	-1.66049100
C	-1.72758800	3.93190600	-1.45564900	C	-0.30858200	2.65679600	-2.92341400
H	-2.72889900	4.33732900	-1.64242100	H	-1.16832900	2.69635100	-3.60064100
H	-1.01108100	4.56742400	-1.98400300	H	0.57321500	2.99103600	-3.47751500
H	-1.68228700	2.92666000	-1.89265200	H	-0.15418200	1.61450000	-2.62491200
C	1.17114800	4.45268800	2.13897600	C	1.26227400	5.36002200	0.58059300
H	1.35564000	3.51167200	2.66181800	H	1.05611600	4.81247400	1.50631700
H	2.01186700	5.12549800	2.34143600	H	2.09208900	6.04887800	0.77097100
H	0.27683200	4.90883900	2.56763400	H	0.38286100	5.95881100	0.33234200

C	2.38567600	3.58096200	0.14372700	C	2.93964300	3.63761900	-0.13807900
H	2.52963400	2.60559900	0.62025800	H	2.83717300	3.15583000	0.83614700
H	2.38580800	3.44791700	-0.94451100	H	3.20415100	2.87287000	-0.87578200
H	3.23496800	4.21989500	0.41056400	H	3.75913700	4.36117800	-0.08486900
H	-0.11916800	1.37627800	0.59854600	H	-0.17543000	0.79612400	-0.24323800
19				20			
Charge=1 Multiplicity = 2				Charge=1 Multiplicity = 2			
O	-1.84577300	-2.27045900	1.85246900	O	-1.89022700	-3.16595900	-1.42121400
O	-0.55560100	-2.07148500		O	-0.66360500	-2.53341700	-1.01258700
	1.24239300			Cu	-0.81257400	-0.80809600	-0.47646500
Cu	-0.22172900	-0.45717200		N	-0.80100500	1.16199100	-0.51260300
	0.43222500			C	-1.93934600	1.73132200	-0.04480800
N	1.56185200	-1.15306300	-	C	0.19746900	1.93644700	-0.96408400
	0.17646900			C	-2.09159200	3.11803700	-0.02638500
C	2.52468600	-0.21785700	-	C	-2.97072900	0.76576900	0.40739600
	0.33724500			C	0.10945400	3.32516200	-0.97943100
C	1.82913400	-2.44416800	-	H	1.08068400	1.41338900	-1.31465700
	0.41100500			H	-3.00222700	3.57071800	0.34748100
C	3.80216600	-0.57055600	-	C	-1.05581800	3.92203800	-0.50057800
	0.77394900			N	-2.62381200	-0.53749400	0.26659900
C	2.10265900	1.16437400		C	-4.21196100	1.12486800	0.93132300
	0.00268100			H	0.93533700	3.91674800	-1.35854400
C	3.08303000	-2.86776600	-	H	-1.16139300	5.00240400	-0.49580000
	0.84711300			C	-3.48745000	-1.50243800	0.61018200
H	1.00954200	-3.12956800	-	C	-5.10418300	0.12125600	1.30940800
	0.22095900			H	-4.48767800	2.16681200	1.04306200
H	4.57336000	0.17881900	-	C	-4.74093900	-1.21341000	1.14465000
	0.90830500			H	-3.15604800	-2.51533000	0.41196800
C	4.07991800	-1.91263700	-	H	-6.07419300	0.38395000	1.71985400
	1.03521000			H	-5.41230900	-2.02069200	1.41543500
N	0.80671100	1.28961600		H	-1.70566400	-4.08963900	-1.17138500
	0.38172900			H	1.61024700	-0.02401400	1.46052600
C	2.95431800	2.27084900	-	C	1.86715700	-0.99439800	1.02624600
	0.02178200			O	1.21867700	-0.99279600	-0.28328100
H	3.26601200	-3.92082700	-	C	3.37422500	-1.17056100	0.91022300
	1.03021000			H	1.41730300	-1.78376500	1.63986500
H	5.06812100	-2.20509800	-	H	1.37579900	-1.85701700	-0.71060900
	1.37650200			H	3.77693400	-1.24235300	1.92885400
C	0.33905200	2.49165500		H	3.58903100	-2.13877000	0.43454300
	0.74987200			C	4.08763800	-0.03547900	0.15135700
C	2.46360200	3.51803100		H	3.63969400	0.05392000	-0.84946300
	0.36000900			H	3.90284100	0.91598300	0.66896900

H	3.98899100	2.16571500	-	C	5.57019200	-0.26676600	0.02731700
0.32577400				H	5.87151200	-1.14354300	-0.54943000
C	1.13285500	3.63458600		C	6.51275600	0.50727900	0.57190100
0.75869200				H	6.20327700	1.38280300	1.14706000
H	-0.70616900	2.52503600		C	7.99244900	0.28296800	0.45920300
1.04094700				H	8.48713200	1.14103200	-0.01450300
H	3.11606700	4.38559400		H	8.45067600	0.16570800	1.44999500
0.34960700				H	8.22272100	-0.61022800	-0.13054300
H	0.71457700	4.58552600					
1.06970200							
N	-1.98217100	0.16371500	-				
0.20473500							
C	-2.21336700	1.13480100	-				
1.16459200							
C	-3.16391300	-0.39108000					
0.05384400							
C	-3.54427100	1.15388100	-				
1.47244800							
H	-1.41587200	1.73801400	-				
1.57103900							
N	-4.13364000	0.17941200	-				
0.68965400							
H	-3.31202200	-1.19979800					
0.75467100							
H	-4.11450200	1.75489300	-				
2.16424000							
C	-5.55122800	-0.17706800	-0.67499700				
H	-6.15208800	0.68480100	-				
0.37382200							
H	-5.86284300	-0.51151400	-1.66767600				
H	-5.70295400	-0.98750900					
0.03911400							
H	-1.63019100	-2.15055300					
2.79444700							
TS20-21				21			
Charge=1 Multiplicity =2				Charge=1 Multiplicity = 2			
C	2.94996200	-2.21228500	-0.49721500	C	3.03674700	-2.07834400	-0.70024000
C	4.26181200	-2.43521600	-0.90803000	C	4.33981200	-2.18168100	-1.17823800
C	5.10087500	-1.33616200	-1.08064800	C	5.09465300	-1.01700000	-1.30521700
C	4.61232300	-0.05201200	-0.83451200	C	4.52962300	0.20849500	-0.95155600
C	3.28980400	0.10113400	-0.42358500	C	3.21829400	0.24122500	-0.47999300
N	2.48132000	-0.97739200	-0.26850500	N	2.49086100	-0.89978400	-0.36502900
H	6.12896300	-1.47221400	-1.40139300	H	6.11452300	-1.05771400	-1.67471500

H	2.24665300	-3.02274100	-0.33957300	H	2.40168300	-2.94932800	-0.57754000
H	4.60928400	-3.44681900	-1.08555200	H	4.74544500	-3.15209100	-1.44159000
H	5.25801900	0.80905900	-0.96088200	H	5.10761500	1.12038900	-1.04399300
H	3.03475900	4.75764300	0.15364800	H	2.67717900	4.82838800	0.38725100
C	2.55740900	3.78347200	0.19248200	C	2.26631400	3.82364900	0.37833900
C	1.23117200	3.66156000	0.60376200	C	0.96218400	3.58889400	0.81033700
C	3.27661700	2.64153900	-0.16451600	C	3.05001500	2.75580100	-0.06298700
C	0.65954800	2.39200000	0.63505900	C	0.47631600	2.28364700	0.77943200
H	0.64699600	4.52680600	0.89658700	H	0.32966700	4.39474600	1.16565700
C	2.64523400	1.40039300	-0.10700500	C	2.50278000	1.47388500	-0.06549000
H	4.31090200	2.72541800	-0.47691400	H	4.06770300	2.92860700	-0.39297600
N	1.35108000	1.29973700	0.28343600	N	1.23102700	1.26440700	0.34974100
H	-0.36290400	2.21776800	0.95355300	H	-0.52372500	2.01794100	1.10554000
Cu	0.65733100	-0.53178700	0.27678300	Cu	0.65563600	-0.60733600	0.26474900
O	0.49748300	-2.51395000	1.98024900	O	0.74001900	-2.63662800	2.28256500
O	-0.10842300	-2.33763500	0.66148200	O	0.17644200	-2.50621100	0.94826100
H	0.09799600	-3.36019800	2.25479500	H	0.66022800	-3.60019900	2.41802800
H	-0.95916400	-1.56951800	0.82809500	H	-0.72816300	-2.08030400	1.09721800
C	-2.09896700	0.05418400	-0.35939200	C	-2.03100600	-0.07018900	-0.41658800
H	-1.83683800	1.04433700	-0.76035400	H	-1.75250100	0.92669800	-0.80178800
H	-2.01386600	-0.66599700	-1.18971600	H	-1.98324300	-0.76571600	-1.27234500
O	-1.17716600	-0.27698400	0.68945400	O	-1.13870200	-0.46246900	0.61647600
C	-3.52869200	0.06754100	0.17203700	C	-3.46378600	-0.02311800	0.11395000
H	-3.77246200	-0.92407100	0.57350300	H	-3.73326100	-1.01518900	0.49705000
H	-3.58212700	0.76933500	1.01438000	H	-3.49739000	0.66273700	0.97094700
C	-4.55769100	0.45462900	-0.90874300	C	-4.48212300	0.41381400	-0.95718700
H	-4.28372300	1.43905800	-1.32013000	H	-4.18149600	1.39861200	-1.34876600
H	-4.50446800	-0.25769600	-1.74292000	H	-4.44770400	-0.28222600	-1.80599100
C	-5.96407100	0.50229200	-0.37382800	C	-5.88707100	0.48867300	-0.42218200
H	-6.15007300	1.22981600	0.41908800	H	-6.05437900	1.20520900	0.38495400
C	-6.96823300	-0.27384000	-0.79010800	C	-6.91175400	-0.25242600	-0.85243700
H	-6.77502400	-0.99846200	-1.58406400	H	-6.73776900	-0.96692100	-1.65991500
C	-8.37252000	-0.23476700	-0.26101200	C	-8.31465300	-0.18614600	-0.32208900
H	-9.08913900	0.00320400	-1.05818300	H	-9.02523500	0.08443800	-1.11432100
H	-8.67029600	-1.21033800	0.14574700	H	-8.63795800	-1.16049000	0.06797100
H	-8.48552800	0.51282200	0.53109500	H	-8.40801200	0.55019000	0.48307100
22				23			
Charge=2 Multiplicity = 3				Charge=2 Multiplicity =1			
Cu	-2.06211500	0.63535500	0.55847200	Cu	-0.41670900	-1.86672400	-0.50173200
N	-3.44200400	-0.31801900	1.59205900	N	-1.94610000	-2.26663600	-1.73390000
N	-3.61261900	1.16960100	-0.54040900	N	-0.92267200	-3.63787800	
C	-5.78761500	-0.74543900	1.77151600	0.23734600			
C	-4.70282500	-0.16257400	1.11807800	C	-3.73061600	-3.79976500	-2.17458400
C	-4.25691800	-1.65260500	3.39738500	C	-2.61747200	-3.40374600	-1.43201800

H	-6.39369200	-1.95630600	3.44644300	C	-3.43320800	-1.85634000	-3.56248600
H	-2.17950900	-1.11892000	3.00095700	H	-5.00899300	-3.30751400	-3.83611000
H	-4.04443100	-2.22955100	4.29061900	H	-1.72240300	-0.64641600	-2.97834700
H	-6.79680300	-0.61756800	1.39808200	H	-3.71487400	-1.22856200	-4.40058200
H	-6.84742700	1.91002500	-2.50766800	H	-4.26540500	-4.71033800	-1.93196200
C	-5.93518800	1.70380400	-1.95664900	H	-2.28617900	-6.99702300	
C	-4.71253800	2.21233200	-2.39268800		1.56632700		
C	-5.97916600	0.92092400	-0.80260000	C	-1.89922000	-6.05321900	
C	-3.57080300	1.92199300	-1.65140800		1.19506100		
H	-4.63865200	2.82185600	-3.28645600	C	-0.74501800	-5.49421100	
C	-4.79715200	0.66594000	-0.10835000		1.74072500		
H	-6.92326300	0.51626300	-0.45746300	C	-2.55276500	-5.39048600	
C	-5.55926600	-1.49824300	2.92459600		0.15692100		
H	-2.59168800	2.29106800	-1.93869000	C	-0.29127200	-4.28060600	
C	-3.21853000	-1.04327800	2.69757400		1.23169100		
O	-0.63341400	-0.37167300	1.23769200	H	-0.20341900	-5.98235800	
O	0.63344600	0.37171900	1.23764900		2.54337200		
Cu	2.06211600	-0.63537600	0.55840700	C	-2.03991200	-4.17920500	-0.30844800
N	3.44198100	0.31800700	1.59202900	H	-3.44587000	-5.81926700	-0.28178400
C	4.70282700	0.16253800	1.11813000	C	-4.14579600	-3.01225900	-3.24783900
C	3.21844300	1.04330800	2.69750500	H	0.60146200	-3.79862600	
C	5.78758500	0.74540600	1.77161700		1.61452400		
C	4.79720500	-0.66599200	-0.10828400	C	-2.33475000	-1.51883900	-2.77634400
C	4.25679500	1.65265300	3.39735300	O	0.00184900	-0.26113900	-
H	2.17940500	1.11895800	3.00082100		1.42725100		
H	6.79679600	0.61750200	1.39825400	O	1.31835500	0.28089500	-
C	5.55917200	1.49825400	2.92465500		1.09280200		
N	3.61269500	-1.16966100	-0.54038400	Cu	1.24619700	2.02603600	-
C	5.97925000	-0.92096500	-0.80248800		0.43528600		
H	4.04426100	2.22964100	4.29054900	N	3.10413300	2.47593200	-
H	6.39357100	1.95632200	3.44654100		0.91645700		
C	3.57092600	-1.92204300	-1.65139300	C	3.57653200	3.59684200	-
C	5.93531900	-1.70383300	-1.95654600		0.31812300		
H	6.92333000	-0.51630300	-0.45730900	C	3.87401500	1.79023200	-
C	4.71268900	-2.21236400	-2.39263600		1.77354100		
H	2.59182700	-2.29113400	-1.93871000	C	4.86447200	4.05955100	-
H	6.84758000	-1.91004500	-2.50753400		0.58437100		
H	4.63883900	-2.82187500	-3.28641500	C	2.61349700	4.25396500	
O	0.82023100	-2.05881200	0.03865700		0.59937700		
C	0.97621300	-3.39855400	0.59651400	C	5.16975200	2.19661000	-
H	1.99954500	-3.70200800	0.35605700		2.08252300		
C	-0.03512600	-4.37010700	0.00407100	H	3.41509800	0.90726700	-
H	0.07537700	-5.32534700	0.53338800		2.20636300		
H	-1.05091600	-4.01401500	0.22918100	H	5.24242400	4.95803600	-

C	0.12270200	-4.59973900	-1.51096000	0.11104700		
H	0.06045300	-3.62654600	-2.02109900	C	5.66852300	3.34890000 -
H	1.12541700	-5.00220600	-1.71141800	1.47697600		
C	-0.91655600	-5.53722000	-2.06649300	N	1.40494100	3.64147800
H	-1.95285700	-5.19934100	-1.99675900	0.68372300		
C	-0.65781000	-6.72715200	-2.61582600	C	2.88766300	5.40091900
H	0.38107500	-7.05750300	-2.68247200	1.34432000		
C	-1.68356000	-7.67248200	-3.16807300	H	5.76622700	1.62216400 -
H	-1.50246300	-7.87227100	-4.23209700	2.78253900		
H	-1.64010500	-8.64293000	-2.65706300	H	6.67306200	3.69702600 -
H	-2.69905900	-7.27676200	-3.06374100	1.69620100		
H	0.88034100	-3.33909200	1.68761000	C	0.45896500	4.13687100
H	-0.00681000	-1.61852100	0.42378000	1.49774300		
O	-0.82030200	2.05890200	0.03876500	C	1.90264400	5.91787600
C	-0.97628100	3.39865800	0.59655900	2.18573000		
H	-1.99961200	3.70210600	0.35608300	H	3.85298900	5.88841000
C	0.03507600	4.37018400	0.00409000	1.27647200		
H	-0.07545000	5.32545000	0.53335200	C	0.66747400	5.27617500
H	1.05086200	4.01411100	0.22924700	2.26893400		
C	-0.12270700	4.59973700	-1.51095800	H	-0.47774200	3.58924800
H	-0.06040800	3.62651800	-2.02104400	1.52701900		
H	-1.12542800	5.00216200	-1.71147400	H	2.10207600	6.81012500
C	0.91654300	5.53722100	-2.06649700	2.77091300		
H	1.95285000	5.19937100	-1.99671600	H	-0.12032900	5.64580500
C	0.65778800	6.72712600	-2.61588500	2.91586300		
H	-0.38110300	7.05744900	-2.68258200	H	-0.67952400	0.09187700
C	1.68353400	7.67246200	-3.16812800	5.73360900		
H	1.50246200	7.87222500	-4.23216300	C	-0.96367400	0.68740700
H	1.64004600	8.64292100	-2.65714200	4.85831600		
H	2.69903800	7.27676600	-3.06375800	C	-2.45325900	1.06675900
H	-0.88041900	3.33924100	1.68765800	4.94573800		
H	0.00677600	1.61864900	0.42381000	C	-0.58347600	-0.13207100
				3.57916400		
				H	-0.35704700	1.59912600
				4.89887700		
				H	-2.63198400	2.01087100
				4.41772900		
				C	-3.32814800	-0.02930500
				4.33934500		
				H	-2.73091900	1.23933400
				5.99107200		
				N	-1.63085200	0.18329400
				2.56874300		
				C	-3.05321600	-0.21872900

2.82290000		
H	-4.39125200	0.20097900
4.47036800		
H	-3.15358900	-0.97115500
4.87388300		
O	-1.22930200	-0.30395000
1.24744000		
C	-3.41253600	-1.65795300
2.40150800		
H	-3.32626000	-1.78833500
1.31895900		
H	-2.78668200	-2.40570800
2.89416600		
H	-4.45268100	-1.86110400
2.67958000		
C	-3.92671700	0.75937100
2.01246600		
H	-4.98833400	0.51717300
2.12985400		
H	-3.77171300	1.79115500
2.34443800		
H	-3.68887000	0.70200800
0.94442000		
C	-0.42040700	-1.63091800
3.91635200		
H	-0.28293200	-2.21898300
3.00473500		
H	0.46554400	-1.77495300
4.54521200		
H	-1.27459800	-2.03500500
4.46449600		
C	0.76853700	0.38192000
3.05204000		
H	1.15667300	-0.24048600
2.24049100		
H	0.67290100	1.41577400
2.69944800		
H	1.50306200	0.37229200
3.86436100		
H	-1.21981300	0.52317700
0.73806700		
C	-1.37935200	2.99302200 -
1.49751000		
H	-1.18024900	3.94974800 -

1.00642400
H -0.90542800 3.01280200 -
2.48694900
O -0.71740800 1.98064000 -
0.68254600
H -0.70149300 1.05924100 -
1.14690600
C -2.87453000 2.73557300 -
1.60737100
H -3.04650900 1.76143200 -
2.08556400
H -3.30185900 2.67540400 -
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C -3.59113400 3.83513800 -
2.41954300
H -3.40503000 4.80491300 -
1.93259400
H -3.15177200 3.90103200 -
3.42359200
C -5.07410000 3.59791400 -
2.52941900
H -5.62467600 3.56050400 -
1.58729200
C -5.73901400 3.45137400 -
3.67883800
H -5.18116300 3.50406400 -
4.61646700
C -7.21961700 3.24174700 -
3.80530100
H -7.68259000 4.05675900 -
4.37631100
H -7.44569700 2.31470600 -
4.34861900
H -7.70848200 3.19355500 -
2.82691300
C 2.34954900 -2.92664800 -
0.77433000
H 1.94447700 -3.92599200 -
0.59315400
H 2.22918900 -2.69691700 -
1.84074800
O 1.52423500 -2.01249400
0.00263300
H 1.75852400 -1.07633900 -

	0.27580700 C 3.80935900 -2.84319100 - 0.35185100 H 4.18346000 -1.82563300 - 0.53035100 H 3.87767200 -3.01999700 0.72911500 C 4.69460200 -3.85323800 - 1.11086900 H 4.30360400 -4.86619000 - 0.92853600 H 4.61453300 -3.67890100 - 2.19212700 C 6.13919300 -3.78384800 - 0.69152000 H 6.34267300 -3.99074600 0.36107600 C 7.15851100 -3.50330900 - 1.50809200 H 6.94640500 -3.30962500 - 2.56207800 C 8.60395100 -3.45207200 - 1.10699000 H 9.19273300 -4.19043900 - 1.66637900 H 9.04448000 -2.47081800 - 1.32831400 H 8.73577800 -3.65279600 - 0.03892200
23 Charge=2 Multiplicity =3 Cu -0.36676700 -1.87615000 -0.49869800 N -1.91028700 -2.32261100 -1.70051100 N -0.82686000 -3.64753400 0.26973500 C -3.66955700 -3.89748700 -2.09320500 C -2.55500200 -3.46749100 -1.37189900 C -3.42768500 -1.97219300 -3.51669000 H -4.97847700 -3.45772400 -3.74574500 H -1.73283000 -0.72080700 -2.97629500 H -3.73169500 -1.36437600 -4.36166800 H -4.18223500 -4.81470900 -1.82911600	26 Charge=2 Multiplicity =3 Cu 2.19411400 -0.22725000 0.11676500 N 3.24170100 0.98897200 1.32207200 N 3.75761100 0.17801100 -1.10785200 C 5.22899500 2.30069700 1.55216000 C 4.39909800 1.46231800 0.80547100 C 3.65244700 2.15992500 3.36591500 H 5.48857700 3.29478400 3.44464400 H 1.92181100 0.92179700 2.88941300 H 3.32703000 2.40878000 4.37012000 H 6.15767000 2.67665900 1.13932600

H	-2.11430500	-7.00363300	1.67984000	H	6.87903300	1.15479100	-3.16513000
C	-1.74852100	-6.06074700	1.28548200	C	6.00093100	0.87774900	-2.59012200
C	-0.59185700	-5.47659200	1.79856000	C	5.04053200	0.02158900	-3.12616500
C	-2.43209300	-5.42462600	0.25002700	C	5.82614100	1.37310000	-1.29892100
C	-0.16656700	-4.26480000	1.26139700	C	3.93596400	-0.30682200	-2.34515600
H	-0.02709900	-5.94386500	2.59765900	H	5.14283500	-0.38975000	-4.12438000
C	-1.94607300	-4.21421000	-0.24547900	C	4.69032800	1.00474700	-0.57559300
H	-3.32774500	-5.87330200	-0.16293300	H	6.56994900	2.03187700	-0.86667900
C	-4.11388100	-3.13600400	-3.17363600	C	4.85103500	2.64922000	2.84850400
H	0.72608400	-3.76347000	1.61867000	H	3.16761000	-0.98464700	-2.70010700
C	-2.32615400	-1.60056900	-2.75045400	C	2.87210600	1.33115400	2.56368600
O	0.01106900	-0.28505700	-1.47009800	O	0.63202000	0.20372900	0.96551000
O	1.31090100	0.30212900	-1.14363900	O	-0.47634100	-0.65726300	0.84635400
Cu	1.17149400	2.03267600	-0.45137800	Cu	-1.99711500	0.04969300	0.09042700
N	3.01214900	2.55576900	-0.93417500	N	-3.19724200	-1.07876300	1.23023300
C	3.44021300	3.69540200	-0.33822600	C	-4.42127900	-1.33042900	0.71029800
C	3.80666900	1.90113400	-1.79278700	C	-2.86306700	-1.57190200	2.43074900
C	4.70805300	4.20913800	-0.60732800	C	-5.35859300	-2.08679100	1.41562100
C	2.45276800	4.31473600	0.57966100	C	-4.65408800	-0.73995200	-0.63080600
C	5.08451600	2.35875800	-2.10487400	C	-3.74874300	-2.33383300	3.18901900
H	3.38191900	1.00089700	-2.22512300	H	-1.85560600	-1.33961400	2.75881300
H	5.05051500	5.12270900	-0.13590500	H	-6.34037500	-2.28427400	1.00188200
C	5.53820300	3.53030000	-1.50087800	C	-5.01733000	-2.59028100	2.67094700
N	1.27009000	3.65416800	0.66719700	N	-3.61290200	-0.02579700	-1.12538800
C	2.68138900	5.47367900	1.32152100	C	-5.83350400	-0.89684700	-1.36092900
H	5.70187300	1.80827000	-2.80603600	H	-3.44807300	-2.71144100	4.16021500
H	6.52761100	3.91807800	-1.72236100	H	-5.73680200	-3.17661400	3.23408800
C	0.30652800	4.11182800	1.48271800	C	-3.72031000	0.54426800	-2.33510200
C	1.67755100	5.95219900	2.16341100	C	-5.93774000	-0.30959600	-2.62104600
H	3.62601000	5.99975600	1.25069500	H	-6.66301000	-1.46723400	-0.96003000
C	0.46994000	5.26045400	2.25087300	C	-4.86261400	0.42318900	-3.12135000
H	-0.60574100	3.52460400	1.51757500	H	-2.85824700	1.11368500	-2.66384300
H	1.84141100	6.85330700	2.74605400	H	-6.84792800	-0.42454200	-3.20136500
H	-0.33080600	5.59881600	2.89901900	H	-4.90425700	0.89505100	-4.09693400
H	-0.51495900	0.15460000	5.71440400	H	-1.70088100	5.10974800	2.35990000
C	-0.84469100	0.72556200	4.83873500	C	-1.22346000	4.76284200	1.43740200
C	-2.33973400	1.07203000	4.97000800	C	-1.21276600	5.89433200	0.38943700
C	-0.48739700	-0.10877000	3.56339000	C	-1.94417300	3.46699000	1.00649400
H	-0.25991800	1.65241800	4.84065700	H	-0.19730700	4.49411900	1.71351800
H	-2.55383700	2.01210700	4.44795600	H	-0.31118200	6.49683800	0.53862500
C	-3.21119300	-0.04071600	4.38947800	C	-1.27901000	5.37641500	-1.06150000
H	-2.59066600	1.23973500	6.02283600	H	-2.05515600	6.57314500	0.55512300
N	-1.56078300	0.18646300	2.57451900	N	-1.35631000	3.02965400	-0.30712100
C	-2.97132400	-0.23332000	2.86712400	C	-0.69093400	3.96870000	-1.27696500

H	-4.27409500	0.17432800	4.54561700	H	-0.75291100	6.06261100	-1.73360100
H	-3.00987100	-0.97732100	4.92349900	H	-2.31904900	5.35982900	-1.40660900
O	-1.18408100	-0.30668500	1.24749900	O	-1.37773200	1.78227100	-0.66009500
C	-3.32214000	-1.67913500	2.46135500	C	-0.99521800	3.50482800	-2.70998400
H	-3.26970300	-1.81185900	1.37695600	H	-0.55309200	2.52897600	-2.92154100
H	-2.66930200	-2.41585900	2.93517400	H	-2.07468100	3.45348400	-2.88655500
H	-4.34937500	-1.89703700	2.77405400	H	-0.57585600	4.23203200	-3.41185100
C	-3.87880600	0.72890800	2.07522200	C	0.83269800	3.92271400	-1.03413100
H	-4.93359800	0.47340200	2.22181600	H	1.33929400	4.52027300	-1.79931400
H	-3.72924700	1.76457400	2.39753900	H	1.11009700	4.32255100	-0.05566300
H	-3.66936200	0.66879000	1.00135900	H	1.19210500	2.89112900	-1.10234400
C	-0.30532800	-1.60167500	3.91730600	C	-3.46159100	3.68568500	0.82917800
H	-0.18366400	-2.20124100	3.01109500	H	-3.94247200	2.78269200	0.43835000
H	0.59578100	-1.72997800	4.52774200	H	-3.90919500	3.91336100	1.80236500
H	-1.14343500	-2.00495400	4.48987000	H	-3.68863100	4.51364900	0.15331200
C	0.84942000	0.40610500	3.00009500	C	-1.68572700	2.38813200	2.07111400
H	1.22717000	-0.22848000	2.19315600	H	-2.36867900	1.53886500	1.98001900
H	0.73885300	1.43224900	2.63030400	H	-0.65980600	2.01406800	2.02483300
H	1.59954600	0.41756700	3.79805600	H	-1.86299100	2.82587100	3.05841900
H	-1.23521500	0.51096600	0.72419600	H	1.14517200	-5.43411400	2.09288700
C	-1.47953900	2.91278600	-1.51754000	C	0.80469500	-4.89299200	1.20384100
H	-1.30767500	3.87443600	-1.02580300	C	0.54000200	-5.88240800	0.04941600
H	-1.00640200	2.94665800	-2.50693900	C	1.84758900	-3.80111500	0.90051200
O	-0.78915100	1.91790400	-0.70423400	H	-0.12639600	-4.39315800	1.49516000
H	-0.73202900	1.00057600	-1.17972300	H	-0.49078700	-6.24256000	0.12987100
C	-2.96692900	2.61342300	-1.62768800	C	0.78580700	-5.27000400	-1.34482900
H	-3.11161100	1.63289900	-2.10174700	H	1.17387600	-6.76813300	0.15587100
H	-3.39348300	2.54603300	-0.61901000	N	1.42894000	-3.09802200	-0.36335400
C	-3.71349800	3.68892100	-2.44507000	C	0.57844700	-3.74312900	-1.42922900
H	-3.55207700	4.66635000	-1.96468800	H	0.12419700	-5.73388700	-2.08434900
H	-3.27803900	3.75986600	-3.45044800	H	1.80628100	-5.48796600	-1.67868100
C	-5.18995600	3.41184400	-2.54996300	O	2.04051300	-2.00440800	-0.67431600
H	-5.73777500	3.36873700	-1.60645400	C	1.03283800	-3.23887100	-2.80619300
C	-5.85270100	3.23643800	-3.69658400	H	0.83858900	-2.17096500	-2.93174800
H	-5.29810400	3.29476100	-4.63579900	H	2.09890800	-3.42561700	-2.96602600
C	-7.32746500	2.98636700	-3.81791300	H	0.47484400	-3.77957900	-3.57665900
H	-7.81299500	3.78330900	-4.39564400	C	-0.89491400	-3.34838600	-1.20009100
H	-7.52989100	2.04852900	-4.35195100	H	-1.50065600	-3.73429900	-2.02721100
H	-7.81299900	2.93459800	-2.83805200	H	-1.29583700	-3.75134500	-0.26715700
C	2.41921900	-2.87515000	-0.79196200	H	-0.98597900	-2.25995600	-1.16457400
H	2.03766100	-3.88102400	-0.59634700	C	3.26201200	-4.38347400	0.69193400
H	2.28287400	-2.65911300	-1.85922600	H	3.95783900	-3.59601300	0.38729800
O	1.58278300	-1.97016300	-0.01560800	H	3.61725200	-4.80787600	1.63657800
H	1.78976900	-1.03282300	-0.31313300	H	3.28431000	-5.17459100	-0.06128300

C	3.88098000	-2.75565000	-0.38530100	C	1.86886800	-2.78535400	2.05398400
H	4.23043100	-1.73158100	-0.57605400	H	2.70137500	-2.08168600	1.96277000
H	3.96403200	-2.92160400	0.69636200	H	0.93253800	-2.22409400	2.10285000
C	4.78130900	-3.75186300	-1.14487700	H	2.00857700	-3.32899900	2.99362900
H	4.41299600	-4.77165000	-0.95359800				
H	4.68973400	-3.58558600	-2.22644500				
C	6.22706000	-3.64977800	-0.73634500				
H	6.44231900	-3.84753000	0.31567100				
C	7.23447400	-3.35112500	-1.56123200				
H	7.01115900	-3.16656000	-2.61450900				
C	8.68114300	-3.26700700	-1.17016100				
H	9.28213900	-3.99420300	-1.73118300				
H	9.09845400	-2.27706000	-1.39764900				
H	8.82443800	-3.46123700	-0.10238000				
27							
Charge=2 Multiplicity =3							
Cu	2.03111400	-0.11295100	0.56834600				
N	2.64466300	0.74890000	2.31109100				
N	4.00208300	0.10168400	0.17153900				
C	4.49950600	1.71904000	3.47108100				
C	3.95244900	1.08848900	2.35166000				
C	2.32847000	1.64564100	4.50470400				
H	4.08446900	2.48823200	5.43901500				
H	0.81823100	0.71297600	3.22973500				
H	1.65844500	1.84550100	5.33386100				
H	5.54841600	1.98896300	3.50273300				
H	7.78433200	0.73183100	-0.32760600				
C	6.72265300	0.55146900	-0.19050300				
C	5.97548500	-0.08919900	-1.17715800				
C	6.09071400	0.95482000	0.98383800				
C	4.61747600	-0.29691100	-0.95194300				
H	6.42991400	-0.42498400	-2.10287000				
C	4.72336300	0.71672000	1.14073800				
H	6.66030300	1.44521600	1.76416100				
C	3.67526800	2.00013300	4.55985000				
H	3.99160500	-0.80083600	-1.67825900				
C	1.85149100	1.02032000	3.35489100				
O	0.25672900	0.00343900	1.12712200				
O	-0.59250600	-1.05462300	0.74181300				
Cu	-2.20581300	-0.58618600	0.02525000				
N	-3.05141300	-2.34547400	0.50947600				
C	-4.08982200	-2.70765700	-0.27794100				
C	-2.66195400	-3.14453500	1.51193900				

C	-4.78568500	-3.89686700	-0.04998300
C	-4.40009700	-1.75053600	-1.36887900
C	-3.30875500	-4.34460100	1.79725700
H	-1.80773600	-2.78972100	2.07867700
H	-5.62144500	-4.18351500	-0.67724500
C	-4.39144200	-4.72117600	1.00318700
N	-3.60976700	-0.64706500	-1.40633000
C	-5.40797400	-1.94895300	-2.31430400
H	-2.97216300	-4.96186600	2.62315900
H	-4.92484200	-5.64659200	1.19719500
C	-3.79664800	0.26015400	-2.37756800
C	-5.59981400	-1.00116100	-3.31809100
H	-6.03595800	-2.83108900	-2.27679100
C	-4.77715600	0.12290100	-3.35582600
H	-3.13018000	1.11392000	-2.36226400
H	-6.37847000	-1.14416800	-4.06080600
H	-4.88714000	0.88023700	-4.12424000
H	1.16150400	2.63869700	-5.21922900
C	1.20761700	3.08590100	-4.21992000
C	2.51652800	3.88542200	-4.05090700
C	1.02751100	1.96014700	-3.18346300
H	0.34257900	3.75518000	-4.15140400
H	2.35960700	4.90296800	-4.42372100
C	2.99807000	3.92128200	-2.58521600
H	3.30660900	3.45687700	-4.67693400
N	0.96217800	2.59779100	-1.82945300
C	1.85297200	3.79904100	-1.55572400
H	3.54151300	4.85341000	-2.39117300
H	3.71780100	3.11544800	-2.40005400
O	1.13290900	1.54554600	-0.83773200
C	2.45764300	3.73705600	-0.14688400
H	1.68807200	3.63684200	0.62463600
H	3.16262500	2.90947200	-0.04173200
H	2.99960900	4.67018400	0.03967100
C	0.94412900	5.04744700	-1.61938800
H	1.53063300	5.95328200	-1.42732400
H	0.46036100	5.16491900	-2.59162800
H	0.15777300	4.98109600	-0.86122300
C	2.13748500	0.89788400	-3.34354600
H	1.97890000	0.07076300	-2.64766400
H	2.10814400	0.49452600	-4.36194000
H	3.13814800	1.30317200	-3.17870000
C	-0.32957900	1.27300800	-3.41899800
H	-0.51037800	0.50702300	-2.65611900

H	-1.13697700	2.01221900	-3.37974000
H	-0.35563700	0.78563300	-4.40025600
H	0.29609600	1.51736300	-0.33812800
H	1.85220100	-5.62416700	1.96851500
C	1.55688700	-5.12775400	1.03784300
C	1.72445600	-6.09203000	-0.15469400
C	2.35761200	-3.81155700	0.93845000
H	0.50043600	-4.85923600	1.15900900
H	0.79778100	-6.66278300	-0.27488800
C	2.08476700	-5.37186200	-1.46940900
H	2.50283900	-6.83054200	0.06150800
N	1.99088400	-3.15739600	-0.36382600
C	1.56578100	-3.92576900	-1.58553000
H	1.69544900	-5.93186600	-2.32644000
H	3.17240900	-5.35117100	-1.59937600
O	2.02846300	-1.87176300	-0.49453100
C	2.18358200	-3.26649000	-2.82889400
H	1.79216900	-2.26091500	-2.99014300
H	3.27416100	-3.21243400	-2.74377300
H	1.94593100	-3.87462300	-3.70730900
C	0.02663100	-3.86358200	-1.67625000
H	-0.30020800	-4.30362200	-2.62452300
H	-0.45495900	-4.41286800	-0.86248600
H	-0.30570300	-2.82237500	-1.63331200
C	3.88222400	-4.05208500	0.97158700
H	4.41909500	-3.11035000	0.81798300
H	4.16477800	-4.44778100	1.95307100
H	4.21523300	-4.76512800	0.21414700
C	1.95860500	-2.89827100	2.10713200
H	2.65237600	-2.06217400	2.22526100
H	0.94691800	-2.50434000	1.98093000
H	2.00233800	-3.48130100	3.03287900
H	-4.56111300	5.15956000	0.78409000
C	-4.51618400	4.10353500	1.07064700
C	-4.88314100	3.93666600	2.55980700
C	-3.12459900	3.56998800	0.67594700
H	-5.25609300	3.59165900	0.44372100
H	-5.96536700	3.79307300	2.63938700
C	-4.13700500	2.77187200	3.23841900
H	-4.66282300	4.85518500	3.11277300
N	-3.05472000	2.12786500	1.10226300
C	-3.77006500	1.58948000	2.31578200
H	-4.73765500	2.36719600	4.06012700
H	-3.21269100	3.13603600	3.69916200

O	-2.19877400	1.37623600	0.48164200
C	-2.82732900	0.64613400	3.07955900
H	-2.56138000	-0.23968600	2.50169700
H	-1.89965900	1.15780000	3.35097600
H	-3.32679900	0.32059900	3.99739900
C	-5.02987400	0.83148200	1.84880300
H	-5.54320500	0.40890200	2.71884500
H	-5.73371100	1.48412100	1.32511300
H	-4.76459800	0.00637400	1.18096600
C	-1.97250300	4.34739500	1.34841000
H	-1.01348400	3.87730800	1.11070800
H	-1.95686200	5.37206000	0.96297000
H	-2.07363800	4.40158500	2.43447300
C	-2.96186000	3.64728100	-0.84872700
H	-1.98102400	3.29145400	-1.17228400
H	-3.74415200	3.07151400	-1.35361900
H	-3.06675400	4.69166200	-1.15817400